

Neutron Scattering Symposium 2020

Virtual Meeting 11th - 13th November 2020

Abstract Booklet



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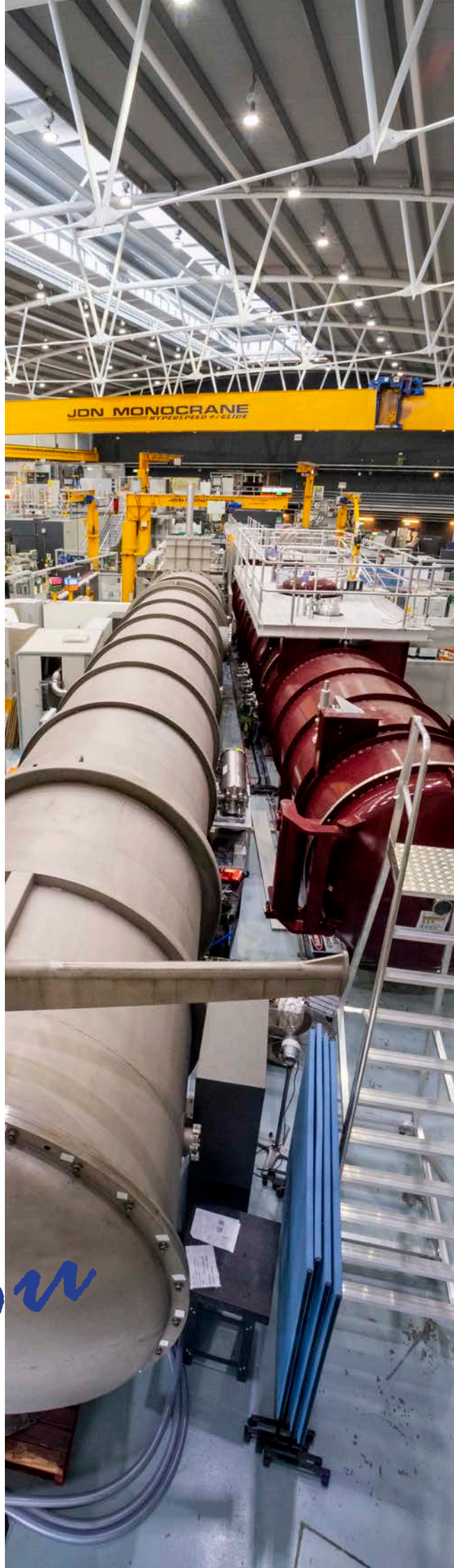
Oral & Poster Prize



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Plenary Speaker



Prof. Dr Andrey Zheludev
Eth Zurich



Andrey Zheludev's research focus is on experimental studies of collective quantum states, excitations and phase transitions in quantum materials, particularly magnetic systems. The main tools are inelastic neutron scattering and neutron diffraction, as well as muon and optical spectroscopies. Andrey Zheludev has been a Professor at the Laboratory for Solid State Physics in the Physics Department since 2009. He was born in 1969 in Moscow, Russia, and grew up in Vienna, Austria. He obtained his Master degree in 1991 at the P. L. Kapitza institute for Physical Problems and the Moscow Institute for Physics and Technology in Russia. Andrey Zheludev earned his PhD in Physics, mention très honorable avec félicitations du jury, from the

Université Joseph Fourier in Grenoble, France, in 1995, having performed his doctoral research at Centre d'Etudes Nucléaires. He joined Brookhaven National Laboratory in the USA 1995. In 2000 he received the Presidential Early Career award for his research on quantum magnetism. In 2001 he became Senior Scientist at Oak Ridge National Laboratory in the USA, and was elected Fellow of the American Physical Society in 2009. Between 2009 and 2010 he headed the Laboratory for Neutron Scattering, Paul Scherrer Institut (PSI), Switzerland.

Keynote Speaker

Dr Hsin-Hui Shen
Monash University



MONASH
University

Dr. Shen is an NHMRC Career Development Fellow at Monash University. She completed her PhD in Physical Chemistry at Oxford University in 2008. Following that, she commenced her postdoctoral research at CSIRO (2008-2011) and received the ARC Super Science Research Fellowship at Monash University (2012-2015). She is a biophysical scientist who can transit between two diverse worlds of biophysics and microbial infections with ease. This is evidenced by her joint appointment with the Biomedicine Discovery Institute, the Department of Biochemistry and Molecular Biology and Faculty of Engineering, the Department of Materials Science and Engineering in Monash University.



Invited Speaker



Dr Gail Iles
RMIT University



Gail has a PhD in experimental physics from the UK and now works as a lecturer in physics at RMIT University. Gail came to Australia in 2014 to work as a scientist at ANSTO where she used neutrons to explore the properties of materials such as structure, magnetism and superconductivity. Gail was an astronaut instructor at the European Astronaut Centre in Germany and holds a medal for extensive time spent experimenting in zero gravity. In 2011, Gail was presented the WISE Champion Award by HRH Princess Anne, for inspiring children, particularly girls, to study STEM subjects.

Prof Bing Li
Chinese Academy of Sciences



中国科学院
CHINESE ACADEMY OF SCIENCES

Dr. Bing Li is currently a full professor in the Institute of Metal Research Chinese Academy of Sciences. He is the Deputy Division Head of the Functional Materials and Devices Division and the principle investigator of the neutron scattering group in Shenyang National Laboratory for Materials Science. His major research involves the preparations and characterizations of novel caloric materials and other emergent energy materials. He emphasizes to utilize neutron scattering and X-ray scattering methods. He has published more than 50 papers on leading academic journals, such as on Nature, Nature Materials, and Nature Communications. He has been recruited into the National Oversea Young Talents Project since 2019. He is now the Chief Scientist of the Key Research Program of Frontier Sciences of Chinese Academy of Sciences.



Dr Floriana Salvemini
ANSTO



Dr Filomena Floriana Salvemini is an instrument scientist on the neutron imaging instrument DINGO. She has recently joined the Bragg Institute, having previously worked as a Ph.D. research fellow at the University of Florence, conducting her activities at the Institute of Complex System (ISC) – National Research Council (CNR) in Sesto Fiorentino. She brings expertise in the area of neutron imaging and diffraction for the investigation of Cultural Heritage, physical metallurgy and archaeometallurgy. In addition she has a strong interest in the application of non-invasive techniques for the study of works of art such as metallographic microscopy, electronic microscopy, ion beam analysis, neutron activation analysis, multi-spectral imaging, X-ray fluorescence, Raman spectroscopy, colorimetry and reflectometry, fiber optics reflectance spectroscopy.

Dr Jon Knott
University of Wollongong



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AUSTRALIA

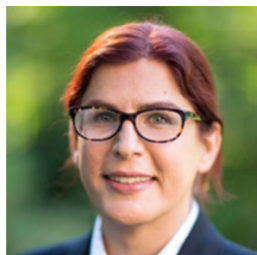
Jonathan Knott is a Research Fellow at the University of Wollongong, where he is co-leading a UOW-ANSTO joint project on additive manufacturing for neutron environment applications. Jonathan was awarded his Bachelor of Engineering (Honours) in Mechatronics, and his Bachelor of Science in Physics from the University of Wollongong in 2008 and 2009 respectively, where he then went on to undertake his PhD candidature – focusing on Applied Superconductivity for power engineering devices. He was Project Manager and Research Fellow on the \$10.5M ARENA-funded Smart Sodium Storage System (S4) Project at the Australian Institute for Innovative Materials before joining the Australian Power Quality and Reliability Centre in 2020.



Invited Speaker



Prof. Lilo Pozzo
University of Washington



Prof. Pozzo's research interests are in the area of colloids, polymers and other soft-matter systems. Her research group focuses on controlling and manipulating materials structure for applications in health, alternative energy and separations. Her group also develops and utilizes new advanced measurement techniques based on neutron and x-ray scattering. Prof. Pozzo obtained her B.S. from the University of Puerto Rico at Mayagüez and her PhD in Chemical Engineering from Carnegie Mellon University in Pittsburgh PA. She also worked in the NIST Center for Neutron Research as a post-doctoral fellow and is currently the Weyerhaeuser Professor of Chemical Engineering at the University of Washington where she has served since 2007. In addition to her research activities, she is also dedicated to improving engineering education with course development in areas of entrepreneurship and service-oriented global engagement.

Dr Gleb Yakubov
University of Nottingham



Dr Gleb Yakubov did his postgraduate research in the University of Mainz and Max Planck Institute for Polymer Research (Germany) and received his PhD in physical chemistry in the area of colloidal probe AFM force spectroscopy. Prior to an academic position at the University of Nottingham (School of Biosciences), Gleb was a Senior Research Fellow in the School of Chemical Engineering at The University of Queensland (Australia), and before then he spent 8 years working in industrial R&D roles in one of the UK-based global fast-moving consumer goods companies. His key expertise area is application of colloidal, soft matter and polymer science principles to the problems in food research, plant biomass biophysics and biomolecular technology. His technical expertise-base is in rheology (flow), tribology (friction & wear), mechanics, and surface characterisation methods, with instrumental capabilities spanning from macroscopic (rotational rheometry) to microscale (soft contact tribology) and nanoscale/molecular characterisation techniques (atomic force microscopy, quartz crystal microbalance with dissipation, ellipsometry, small angle scattering incl. USANS/SANS/SAXS/DLS).



2019 Award Winners



Assoc. Prof. Ric Tabor
Monash University



Rico completed his undergraduate studies at Bristol University in the UK. After a brief period working as a research associate in inorganic synthesis, he returned to physical chemistry at Bristol to complete his PhD, under the supervision of Julian Eastoe, Terence Cosgrove and Peter Dowding.

In 2009, Rico came to Australia as a post-doc, initially at the University of Melbourne, where he worked on unravelling the problems of dynamic and fundamental forces in deformable droplet and bubble systems. In July 2012, he started as a lecturer in physical chemistry at Monash University.

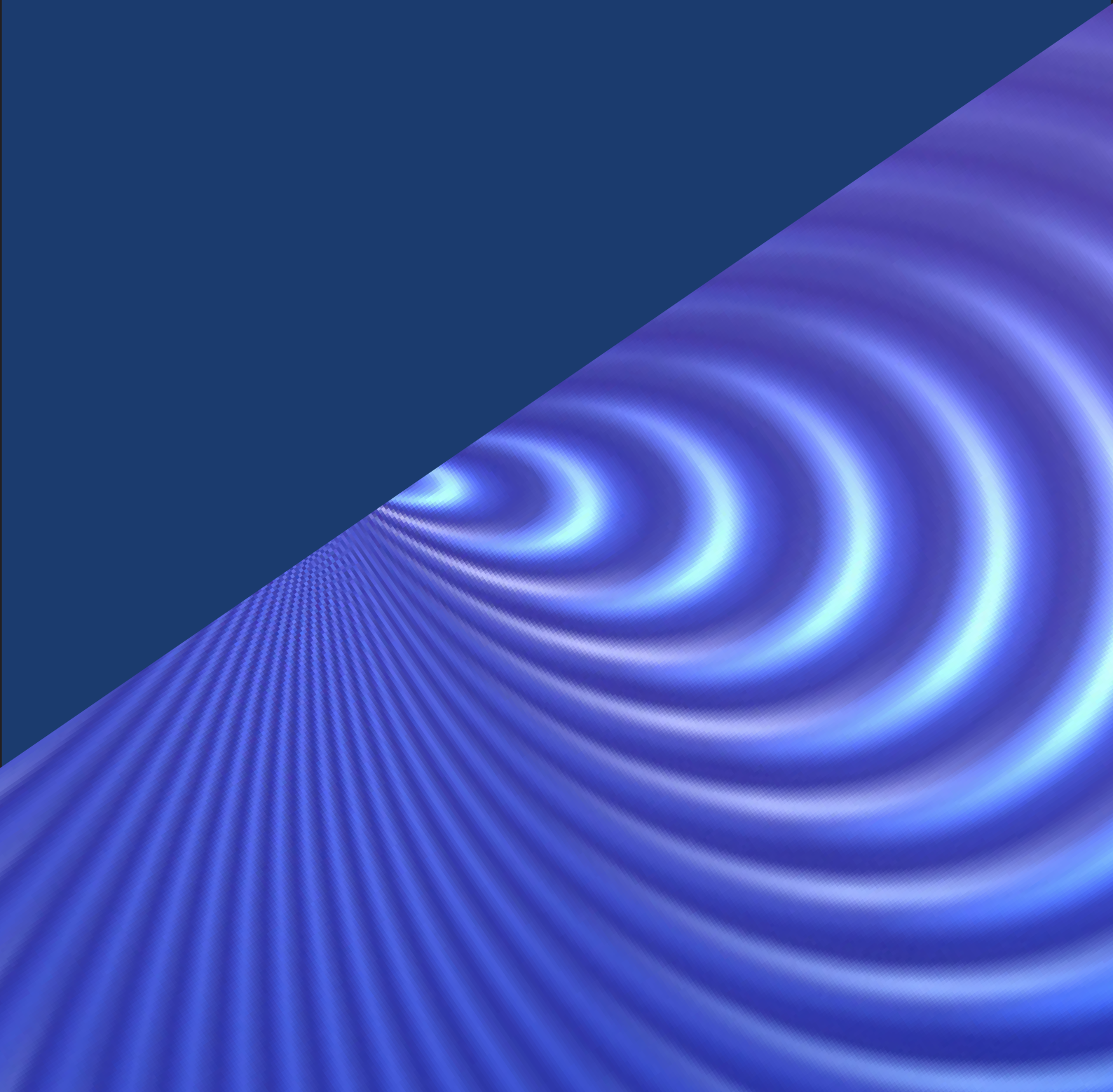
Prof Vanessa Peterson
ANSTO



Prof Vanessa Peterson is a Senior Principal Research and Neutron Instrument Scientist at the Australian Centre for Neutron Scattering (ACNS) where she co-operates the Wombat and Echidna neutron powder diffractometers. Vanessa holds a Professorial Fellowship at the University of Wollongong and leads the "Energy Materials" research project from within the ACNS. Vanessa specializes in atomic and molecular scale material characterization to understand materials function, particularly using real-time neutron and X-ray scattering. Vanessa obtained her PhD in 2004 from the University of Technology, Sydney, in conjunction with the neutron scattering group at ANSTO. She continued to expand her neutron scattering research at the National Institute of Standards and Technology's Center for Neutron Research in conjunction with the University of Maryland in the USA, before returning to Australia to the University of Sydney in 2006. Vanessa joined the ACNS in 2007, where alongside colleagues she commissioned the two neutron powder diffractometers. Vanessa has focused primarily over the last decade on studying materials central to sustainable-energy systems, including materials for battery, fuel-cell, and gas separation technologies, and she has pioneered neutron and X-ray scattering techniques to study these materials that provide a fundamental understanding of how to improve them.



Plenary Speaker



Arguably, materials magnetism has benefited from neutron scattering experiments more than almost any other field of condensed matter physics. For this there are good reasons. Neutron diffraction directly couples to the magnetic order parameter, even in complex structures with non-trivial propagation vectors. In many cases it is the only experimental tool available to study the latter. At the same time, inelastic neutron scattering has a large contribution from elementary excitations (spin waves). Using modern neutron instrumentation measuring magnon dispersion relations, structure factors and lifetimes has become almost ridiculously easy. Once we know the ground state and elementary excitations, we know almost all there is to know about a magnetic material. In this way, a comprehensive neutron scattering investigation has definitively “closed the book” on many a problem in magnetism. At least, such was the state of affairs in **quasiclassical** magnetism...

The focus today is on **quantum** magnets. To understand the beautiful and complex physics of these deceptively simple systems we need neutron scattering more than ever. Unfortunately, its advantages are less overwhelming than in the quasiclassical case. First of all, many of the more interesting quantum magnets do not have any dipolar order in the ground state, making neutron diffraction essentially useless. Some systems remain truly disordered even at $T=0$ due to zero point spin fluctuations. Others, such as spin nematics, have order parameters that are invisible to neutron scattering. Spin liquids, presently the “hottest” topic in quantum magnetism have peculiar topological order that entirely eludes detection. The situation with excitations is no better. Elementary excitations in quantum spin systems are often not magnons but exotic quasiparticles with fractional quantum numbers. Magnetic inelastic scattering is of course present, but is a diffuse and often rather featureless multiparticle continuum. Dispersion relations of the actual elementary excitations are inaccessible.

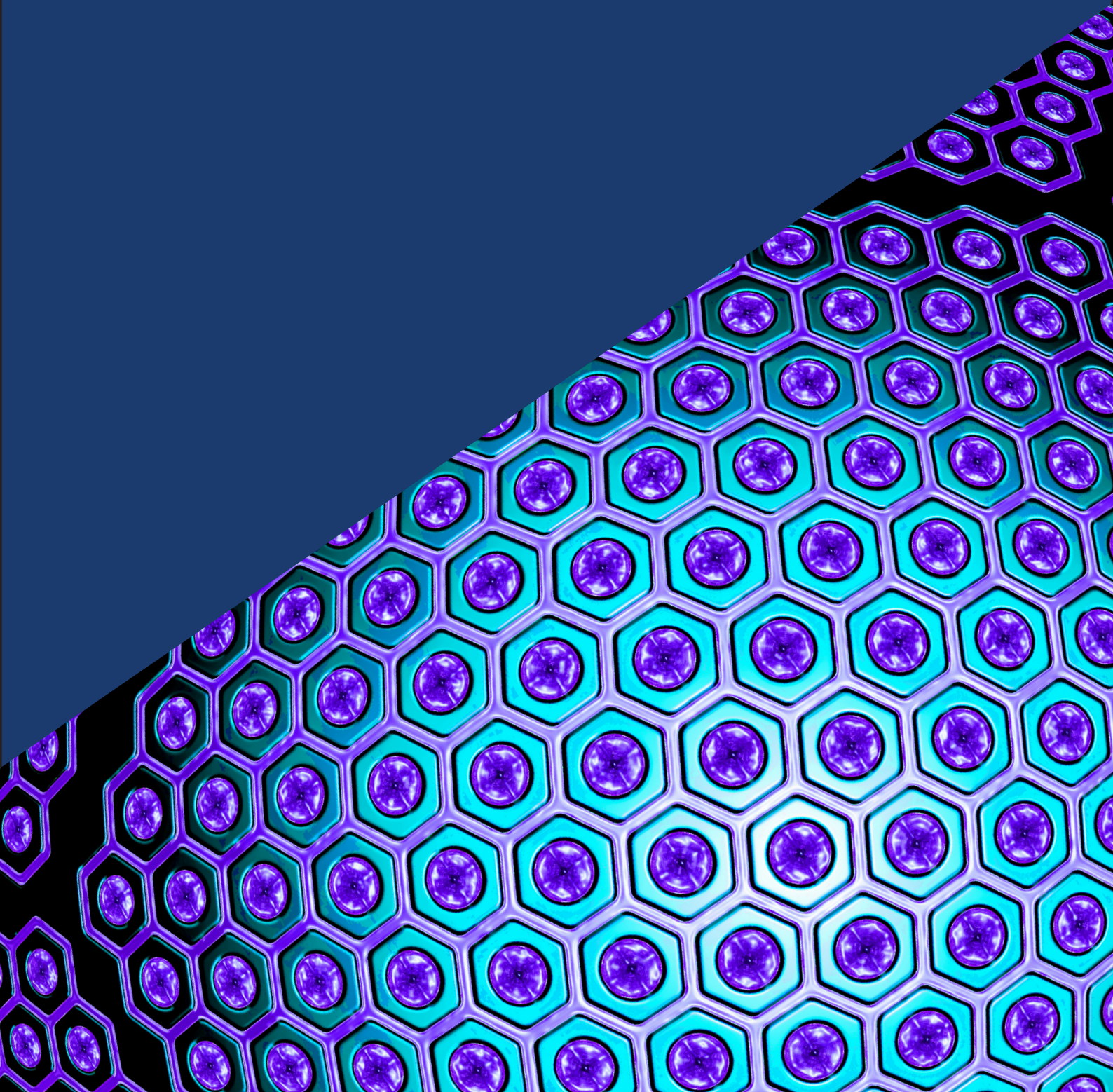
Does this mean that neutron scattering is useless in the study of quantum magnetism? Of course not! It only means that neutrons are no longer the ultimate silver bullet and should be intelligently combined with other methods: magnetic thermodynamics, local probe techniques (NMR, μ SR), light scattering and even dielectric measurements. For correct data interpretation quantitative theoretical numerical modeling of neutron spectra becomes crucially important. So does sample quality and a good control of materials-related issues. Neutron experiments themselves need to be taken to a new level in terms of resolution, intensity and quantitative accuracy.

My talk will be divided into two parts. In the first half I will illustrate the above-mentioned points with some recent examples of successful (and not-so-successful) neutron scattering studies of novel quantum spin systems from literature. In the second half I will present a more in-depth case study from my own research: the investigation of “presaturation” phases in frustrated quantum ferro-antiferromagnets and the ongoing search for the quantum spin nematic state.

Abstract ID # 125

**Prof
Andrey Zheludev**

Advanced Materials *Oral*



Morphological transitions in aqueous surface active ionic liquid influenced by additives investigated through SANS

Designing microscopic interactions judiciously in the amphiphilic systems with added additives is advantageous in order to design various morphologies. Apart from the biological relevance, ease of formation, and long-term stability, catanionic systems could form various morphologies including vesicles, which are the best alternatives to liposomes and niosomes and are potentially the best ever cavity to carry the drug molecules within its cage/bilayer. In a quest for the best catanionic system to sequester functional molecules, herein we have investigated the concentration/composition induced morphological transitions in the catanionic systems comprising of surface-active ionic liquids (SAILs) and various inorganic and organic electrolytes. The variables studied for the phase transition and the shape and size of the aggregates includes; alkyl chain length and head group structures of the SAILs and the concentration and structure of the additives. We used various spectroscopic, microscopic and scattering techniques to determine the size and shape of the aggregates including SANS. The micelle to vesicle transition through added additive is investigated by SANS. The size of micelle, vesicle and bilayer thickness of vesicle is also determined through SANS. For the first time, we used fluorescence resonance energy transfer (FRET) to determine the size of the aggregates and prove the significance of this technique by correlating data with SANS data. This work could be of interest in the field of drug delivery as the possible new age nanocarriers.

*Abstract ID # 41
Advanced Materials*

Monika Jain

Investigating the Aqueous Swelling and Stability of Plasma Polymerised Acrylic Acid Films

Plasma polymer films have been deposited on planar surfaces for a wide variety of applications, such as controlling cell growth or adding anchor molecules for biosensors. They can however also be deposited onto three dimensional objects, such as tissue engineering scaffolds, biomedical implants or 3D printed devices. Coating three-dimensional objects however is more complex as greater monomer fragmentation occurs closer to the electrode. It is therefore important to understand the properties of the plasma polymer films deposited at varying distances from the electrode. The use of plasma polymer films in biomedical applications also requires suitably stable films under physiological conditions, which will also be influenced by the distance from the electrode. Significant changes in film properties in aqueous conditions have serious implications on the incorporation of these films into a number of devices.

Acrylic acid is a commonly used monomer for plasma polymerisation to produce negatively charged carboxylic acid terminated surfaces, which have been used for a number of biomedical applications by manipulating cell growth. To gain a greater understanding of the spatially dependent behaviour of plasma polymerized acrylic acid (ppAAc) films deposited in our custom-built stainless steel T-shaped reactor, ppAAc films were deposited at varying distances from the electrode (3 – 19 cm) at different deposition powers (5 – 80 W). The surface chemistry was analysed with X-ray photoelectron spectroscopy while the film thickness was determined using spectroscopic ellipsometry. Film swelling of a selected group of samples was investigated with neutron reflectometry. Aqueous stability was investigated via immersion in Milli-Q and phosphate buffered saline. The film thicknesses and aqueous stability decreased while the carboxyl group concentrations increased as the distance from the electrode increased and/or the deposition power decreased due to reduced monomer fragmentation further from the electrode and at lower powers. For films deposited 11 cm from the electrode, complete film loss occurred at 20 W with film swelling at 30 W but no swelling at 40 W. This work highlights the importance of having a spatially well characterised plasma reactor to enable the deposition of plasma polymer films with the desired properties, which has significant implications on the incorporation of these films into a number of applications.

*Abstract ID # 2
Advanced Materials*

Karyn Jarvis

Effect of molybdenum on the precipitation in ferritic niobium-containing steels produced by strip casting

Molybdenum (Mo) is often alloyed into the steels containing niobium (Nb), in order to enhance the formation of harder microstructures, such as bainite and acicular ferrite, and denser and finer precipitates. However, the effect of Mo on the nano-precipitates formed in the ferrite of Nb steels is still subject to debate, mostly due to its experimentally challenging nature. In addition, direct strip casting is a revolutionary casting technique that integrates casting and subsequent rolling together with rapid solidification and cooling rates, which not only simplifies the process, but also confers superior energy-saving as compared to conventional alloy thermomechanical processing. In this work, therefore, we have studied the effect of Mo on the precipitation in the ferrite of a Nb-containing micro-alloyed steel produced by strip casting using various advanced characterisation techniques. Isothermal ageing treatments were carried out at 650 °C up to 10,000 s to form precipitates, and the strength was measured using shear punch test. Transmission electron microscopy (TEM) observation showed that precipitates were formed along dislocations in both steels with and without Mo. Atom probe tomography (APT) analyses revealed that the addition of Mo increased both size and volume fraction of solute clusters after short ageing times, which provided a much higher cluster strengthening. Precipitation of Nb-rich carbonitrides were found after longer ageing treatments. However, no significant Mo was observed to segregate to the precipitate. Small-angle neutron scattering (SANS) results indicated that the addition of Mo reduced the average precipitate size. X-ray diffraction (XRD) results suggested that this was attributed to the higher dislocation density that increased the number of nucleation sites.

This work has been published in:

L. Jiang, R.K.W. Marceau, B. Guan, T. Dorin, K. Wood, P.D. Hodgson, N. Stanford, The effect of molybdenum on clustering and precipitation behaviour of strip-cast steels containing niobium, *Materialia* 8 (2019) 100462.

Abstract ID # 42
Advanced Materials

Lu Jiang

In the present work we investigate the important issue of the structure and dynamics of smaller ions in oxides and the resulting impact on its functional properties. For this purpose, we selected a 7% Li-doped BaTiO₃. Li is a vital ingredient in novel energy storage technologies such as Li-ion batteries. The smaller Li-ion can influence the structural stability, homogeneity, local environment, and dynamic behavior of the host lattice, affecting and optimizing the dielectric and multiferroic properties of novel polar functional materials [1-2]. However, the Li-ion positions and dynamics in functional materials are not completely understood, controversially discussed and are the subject of extensive ongoing research [3]. Furthermore, sample inhomogeneity due to Li migration to the grain boundary and/or development of multiple phases complicates the elucidation of the structure-property correlations that may lead to incorrect interpretations [4]. The selection of BaTiO₃ as the host lattice is due to materials based on this being considered as the alternative to the piezoelectric lead zirconate titanate, citing environmental issues [5]. BaTiO₃ also crystallizes in a simple perovskite structure and Li ions can be effectively doped into it at lower doping levels. Very recently, field-dependent electric polarization measurements on BaTiO₃ exhibited a polarization–electric field double hysteresis loop upon Li doping [4]. These drastic changes to the electric polarization, related to the doping poses a good test case for the investigation of the Li-induced defect structure model and its influence on the functional properties. To elucidate the above structure-property correlations, we combined several techniques, such as neutron powder diffraction electron microprobe associated with the wavelength-dispersive spectroscopy, ⁷Li nuclear magnetic resonance spectroscopy (NMR), electron paramagnetic resonance (EPR), electric polarization measurement, and theoretical calculations based on density functional theory [6].

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[2] Y. Liu et al., Appl. Phys. Lett. 91, 152907 (2007).

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*Abstract ID # 105
Advanced Materials*

**Narendrakumar
Narayanan**

Kinetic Analysis of Oil Exchange between Surfactant-Stabilized Emulsions Using Time-Resolved Small Angle Neutron Scattering

Emulsion systems are dynamic and several physical mechanisms can lead to mass transport between droplets (e.g. coalescence, diffusion, micelle-driven). Understanding how oil exchanges between emulsions is also critical to developing applications such as new drug-delivery vehicles and emulsion polymerization processes. Researchers have aimed to fundamentally examine mass transport between stabilized emulsions using characterization techniques such as differential scanning calorimetry, microscopy, pulse gradient NMR, and turbidity measurements. However, all of these require the use of dissimilar oils and/or labeling droplets with fluorescent molecules. Here, we take advantage of large differences in neutron scattering length density between hydrogenated and deuterated versions of alkane oils to use time-resolved small angle neutron scattering to directly examine mass transport between emulsions with identical chemical compositions. We specifically examined mixing between alkanes in oil-in-water emulsions stabilized by anionic (i.e. sodium dodecyl sulfate) and non-ionic surfactants. Fully deuterated and partially hydrogenated hexadecane emulsions with equal contrast relative to the solvent were prepared identically (e.g. sonication) and subsequently mixed to monitor oil exchange kinetics. As oil exchanges between droplets over time, a decrease is observed in scattering intensity due to contrast-matching conditions between the solvent and the fully-mixed oil phases. When emulsions are ideally mixed, minimal scattering is detected. This talk will summarize findings of measurements of mass-transport for emulsion systems with a large number of variable parameters including surfactant concentration, surfactant type, temperature and oil-type. Multiple physical mechanisms are suggested to play important roles in controlling transport in emulsion systems.

*Abstract ID # 117
Advanced Materials*

Lilo D Pozzo
Invited Speaker

Biological Systems

Oral



Resolving the DNA interaction of the MexR antibiotics resistance regulatory protein

Small Angle scattering is a powerful tool for analysing the shape and conformational changes of macromolecules; in particular, protein-DNA complexes need to be highly dynamic in order to be able to respond to external factors for the regulation.

Acquired multidrug resistance (MDR) in pathogenic microbes is a worldwide threat to human health. Several MarR-like proteins regulate the expression of efflux pumps, which are multiprotein self-assembly complexes actively extruding high toxic compounds to the host organism. Since incapacitating the repressor protein leads to continuously high production of the efflux proteins and thus increased survival for the bacteria, there is high mutational pressure for acquired MDR; MexR is a crucial member of the MarR family. According to the DNA binding site for MexR dimer appears to involve an inverted repeat of the sequence; furthermore, it is possible to identify two closely located binding fragments, dubbed as PI and PII. In this work, we will use SANS to reveal the structure of the protein-DNA complex of MexR with its PII and entire (PI+PII) operator regions. This analysis is an essential step for the comprehension of the binding of MarR family proteins with DNA because very few of those proteins have crystallised with DNA and none with two dimer sites. The ongoing analysis will apply to the entire MarR family, and thus provide critical knowledge on pathogenic bacteria, of relevance for clinical understanding and future drug design.

Abstract ID # 7
Biological Systems

Francesca Caporaletti

Protein deuteration extending structural characterisations by Small Angle Neutron Scattering with Contrast Variation

Protein deuteration enables unique applications of neutron scattering to the life sciences, at both low and high resolutions. In recent years, the National Deuteration Facility at ANSTO have developed and published a robust and efficient method of recombinant protein deuteration.[1] Utilising this method enables us to routinely collaborate with life scientists by removing the difficulty of biomolecule deuteration from their needs for sample preparation to make best use of neutron scattering.

In this presentation I will highlight the essential role of protein deuteration in the structural characterization of previously poorly characterized “suppressor of copper sensitivity” proteins, as recently published.[2] Using this, and more recent work in progress, I will illustrate the value of small angle scattering as a complementary method to high resolution techniques so as to including disordered-to-ordered transitions that are frequently the basis for functional mechanisms in life and disease. Other applications of protein deuteration, for neutron reflectometry, neutron crystallography, and nuclear magnetic resonance, will be briefly explained.

References

[1] Robust high-yield methodologies for 2H and $2\text{H}/^{15}\text{N}/^{13}\text{C}$ labeling of proteins for structural investigations using neutron scattering and NMR

AP Duff, KL Wilde, A Rekas, V Lake, PJ Holden

Methods in enzymology (2015) 565, 3-25

[2] Disulfide isomerase activity of the dynamic, trimeric *Proteus mirabilis* ScsC protein is primed by the tandem immunoglobulin-fold domain of ScsB

EJ Furlong, HG Choudhury, F Kurth, AP Duff, AE Whitten, JL Martin

Journal of Biological Chemistry (2018) 293(16), 5793-5805

Abstract ID # 37
Biological Systems

Anthony Duff

A variety of biological processes occur on cell membranes. The complexity of biological membranes makes the determination of their exact composition in a cell quite difficult. A number of simpler model membrane systems have been developed to customize the membrane size, geometry, and compositions with greater precision. In recent years, model membrane systems have been explored and investigated for their interactions with nanocarriers, drugs and antibiotics. Understanding these mechanisms of interactions is essential to the design and development of new drugs and efficient delivery systems. In this talk, I will demonstrate the use of model lipid membranes to understand the biological mechanisms in two different fields.

i) Design of cubosomes for glaucoma drug delivery. Glaucoma is the leading cause of irreversible blindness. It is associated with progressive loss of retinal ganglion cells (RGCs) undergoing apoptosis. We have used cubosomes for glaucoma drug delivery due to their biocompatible constituents and high loading potential for drugs. To enhance the detection of apoptotic cells in glaucoma, cubosomes were first modified with Annexin V. The interactions of Annexin V-containing cubosomes with the apoptotic model and cellular membranes were investigated. After that, we used Annexin V-containing cubosomes as an active targeted delivery system to deliver neuroprotective drugs to the damaged RGCs in vivo. Biophysical studies further revealed that 17% drug loaded cubosomes with Pn3m symmetry have shown better in-situ and in-vitro cell penetration effects than other formulations with Im3m symmetry. This data has important implications for future design and formulation of nanoparticles for therapeutic applications.

ii) Interaction of antibiotics with bacterial outer membranes. “Superbugs” are responsible for more than 35,000 deaths and nearly 3 million illnesses each year. Superbugs can evade last-line antibiotics and the host immune system during a life-threatening infection. Studies have reported that superbugs rapidly adapt their bacterial membrane to circumvent antibiotic and immune killing. We have used neutron reflectometry to characterise the golden staph and gram-negative bacterial membranes, and found that the packing, organisation and density of lipids in the membrane impacted the mechanism of action of antibiotics.

*Abstract ID # 132
Biological Systems*

Hsin-Hui Shen
Keynote Speaker

Advancements in the provision of Deuterated Lipids for Neutron applications from the National Deuteration Facility

Molecular deuteration significantly increases the options for structure-function investigations using neutron scattering and diffraction techniques. Chemical deuteration activities, where catalysed $1\text{H}/2\text{H}$ exchange is followed by custom chemical synthesis, have led to diverse neutron scattering and reflectometry studies previously hampered by the lack of appropriate scattering contrast in multi-component samples. Deuteration of phospholipids is a common practice to elucidate membrane structure, dynamics and function, by providing selective visualisation in neutron scattering. Although analogous deuterium (2H) and hydrogen-containing (1H) molecules have similar physicochemical properties, these isotopes of hydrogen result in vastly different neutron scattering signals. Over the past few years the National Deuteration Facility (ANSTO) has increased its synthetic capability to produce complex deuterated molecules including lipids and phospholipids. Such synthetically challenging molecules are perdeuterated phytantriol¹, tail deuterated POPC, and perdeuterated POPC.² Phytantriol is an interfacially-active lipid that is chemically robust, non-digestible and forms particles with internal bicontinuous cubic phase structures (cubosomes) when dispersed with non-ionic surfactants at physiological temperatures. The tail-deuterated POPC, perdeuterated POPC and tail-deuterated GMO isotopologues would also provide suitable contrast for many neutron experiments and so these have been also our synthetic targets. Recently neutron reflection was employed to investigate the impact of phospholipid saturation (POPC-d64) and presence of cholesterol in cell model membranes on LDL and HDL lipid exchange and removal processes.³ Neutron reflection data that distinguish the effect of phospholipid acyl chain saturation and the presence of cholesterol on the ability of lipoproteins to exchange lipids to/from model membrane will be presented.

References:

- (1) Yepuri, N. R.; Clulow, A. J.; Prentice, R. N.; Gilbert, E. P.; Hawley, A.; Rizwan, S. B.; Boyd, B. J.; Darwish, T. A. J. *Colloid Interface Sci.* 2019, 534, 399.
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- Keywords: Deuteration, neutron reflectivity, contrast variation
Submission for ? oral or ? poster presentation

Abstract ID # 76
Biological Systems

Rao Yepuri

Biomedicine & Food Science Oral



Neutron scattering for the study of casein gel microstructure during digestion

An understanding of the structural factors that affect food digestion kinetics is important for establishing the relationship between their structure and function. To assess the effects of structure on mechanical breakdown and digestibility by pepsin enzyme during gastric digestion, casein gels with an identical composition, but differing by the coagulation mode, were characterized and submitted to simulated in vitro gastric digestion. Rennet-induced (RG) and transglutaminase-induced acid (TG) gels were made and digested in two different solvents- H₂O and D₂O. The structural changes were assessed during simulated gastric digestion by ultra-small (USANS) and small angle neutron scattering (SANS).

The different structures of RG and TG reveal distinctive breakdown behaviours over a hierarchy of length scales (nano- to micro). Different functional properties of casein gels, such as gel strength, elasticity, brittleness, resistance to shear and sensitivity to the acidic environment of gastric phase, obtained by scanning (SEM) and transmission electron microscopy (TEM), contributed to the differences in gel disintegration and gastric digestibility. Despite the higher gel strength and thus higher number of larger gel particles entering the gastric phase following mastication, the porous microstructure of RG provided a larger surface area and thus higher simulated digestibility compared to TG. The effect of acidification is clearer with RG, wherein the local compactness of each gel consequently drives its porosity and pepsin accessibility. On the other hand, pepsin has a limited diffusion capability inside the TG structure due to its fine stranded network; however, the brittle structure of TG is more affected by mechanical shear during the gastric phase, causing particle erosion. In a similar manner, gels made and digested in D₂O had a higher level of mechanical breakdown due to their brittle structure: initially led by the fracturing of particles with a larger surface area, this increases the levels of solubilised protein, small peptides and amino acids.

Here, we report the first USANS and SANS study to monitor structural changes of a casein gel both in H₂O and D₂O during simulated in vitro gastric digestion. We show that solvent (H₂O and D₂O) and gel type (RG and TG) affects digestion components: mechanical shear, enzymatic hydrolysis and the effect of acidification.

*Abstract ID # 20
Biomedicine &
Food Science*

Meltem Bayrak

Oil-in-water emulsion system stabilized by emulsion droplets coated with whey protein microgels

Structurally designed emulsions are a developing group that is likely to find increasing utilization within the food industry because of their potential advantages over conventional emulsions. A novel droplet-stabilized (DS) emulsion system emulsified with casein micelles has been previously reported [1]. However, the mechanism of DS emulsion formation, physicochemical properties, and stability are not yet been fully explored. In the present study, heat-induced whey protein microgel (WPM) particles were used as an alternative emulsifying agent. The structure of WPM particles on the formation and physicochemical properties of the primary (PE) and the DS emulsions was investigated [2]. WPM particles were prepared by heating 4 wt% whey protein isolate solution in the presence (PB) or absence (NPB) of 10 mM phosphate buffer at pH 5.9, 85°C for 45 min, followed by washing, centrifugation, and micro-fluidization. The PE coated with WPM was homogenized using 3 passes at the pressure of 250/50 bar. DS emulsions were prepared by mixing (at 30000 rev/min for 2 min) 10 wt% oil with 10, 30, or 60 wt% PE. The structure of WPM particles and emulsions were analyzed by dynamic light scattering, confocal light scattering microscopy (CLSM), transmission electronic microscopy (TEM), and the combination of small and ultra-small angle neutron scattering (SANS and USANS). The results showed that the WPM particles produced in the absence of phosphate buffer (WPM-NPB) were smooth spherical particles, giving a surface fractal dimension of 2.0 and a hydrodynamic diameter of 270 nm. However, WPM particles made in the presence of phosphate buffer (WPM-PB) were rough spherical particles with a surface fractal dimension of 2.3 and a hydrodynamic diameter of 290 nm. Particle fragments present in the WPM-PB dispersion, resulted in their competitive adsorption onto the surface of the DS emulsions; reducing the adsorption of PE droplets. For the PE coated with WPM-NPB particles (PE-NPB), flocculation due to protein bridging and protein intramolecular interaction, lead to a network with a fractal dimension of 2.7. For the DS emulsions stabilized by PE-NPB, the interfacial layer thickness of DS emulsion droplets increased with the increase in the concentration of PE as observed by CLSM, whereas the size of DS emulsion droplets decreased. A fractal network consisting of adsorbed PE droplets on the interfacial layer of DS emulsion was observed by TEM and measured by USANS with a fractal dimension of 3.0, suggesting a very rough interface. These results suggest that both the structure of the interfacial layer and the size of the DS emulsion is dependent on the concentration of the PE used.

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*Abstract ID # 6
Biomedicine &
Food Science*

Lirong Cheng

Hyaluronic acid-poloxamer thermosensitive hydrogels studied by Small-Angle Neutron Scattering (SANS) and rheology: from nanostructure to biomedical applications

Poloxamer (P)-based hydrogels have been used as drug carrier due to its low toxicity and ability to control drug release, mainly due to their ability to self-assemble in micelles and supramolecular structures with different phase organizations in response to physiological temperature and additives such as drugs, salts and other polymers. These features favor their parenteral administration associated to hyaluronic acid (HA) for improving hydrogels mechanical properties and to develop biocompatible formulations. Hydrogels formulations with P407 (15% or 30% w/w), HA (0.5% w/w) and the local anesthetics ropivacaine (RVC) or bupivacaine (BVC) (0.5% w/w), isolated or in binary systems with P338 (P407 15% + P338 15%), were prepared in D₂O and measured in V16 SANS (HZB, Berlin-Germany) at 25 °C, 37 °C and 40 °C. For rheological analysis, samples were analyzed against frequency sweep and temperature interval from 10 to 50 °C to determine viscous (G'), elastic (G'') moduli and sol-gel transition temperature ($T_{sol-gel}$). SANS results revealed all P407 15% systems were organized as lamellar structures, with decreased lattice parameters according to temperature increase. P407 30% and P407 15% + P407 15% samples present cubic and hexagonal structures, indicating both phases organization coexistence. SANS data showed that BVC decreased the lattice parameter in 3 % after incorporation into P407 30%, and 6% in P407 30% + HA at three temperatures. As BVC is more hydrophobic than RVC, it is probably maintained inside micellar hydrophobic core and expelling water molecules, resulting in a stable structure even at 40 °C. For P407 30% samples, HA decreased in 3% the lattice parameter at 25 °C but presented increased particle sizes (10 nm). Possibly, HA hydrophilic chains act as scaffolds around P407 supramolecular aggregates, stabilizing their phase organization. For binary systems, no structural changes were observed, since for P407 15% + P338 15% hydrogels showed similar lattice parameter to P407 30%. Whereby P338 is more hydrophilic than P407, with a longer polyethylene oxide hydrophilic chains, is possible to form highly hydrated gel structure. These structural differences result from the material properties: the presence of drugs RVC or BVC in P407 30% did not shift the $T_{sol-gel}$ (~22 to 23°C), but increased the G'/G'' relationship from 31 to 47-fold, which shows enhanced structural interaction among polymeric chains. HA, on the contrary, reduced the $T_{sol-gel}$ value until ~21 °C and increased G'/G'' to 38-fold when incorporated to P407 30%. P407 15% + P338 15% system displayed high $T_{sol-gel}$ (~28 °C) and G'/G'' (x40) values. Therefore, as it is seen in our work, the addition of additives can promote mechanical and structural changes, enabling the design of the best supramolecular structure and mechanical properties for controlling drug release kinetics.

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*Abstract ID # 88
Biomedicine &
Food Science*

**Anderson
Ferreira Sepulveda**

Mixed gamma/neutron field in-vivo dosimetry using Metal-Oxide Semiconductor Field-Effect Transistor for Accelerator-Based Boron Neutron Capture Therapy

Introduction

BNCT systems have their specific neutron energy spectra extending from thermal to fast neutron (FN) range of up to a few MeV and γ contamination. Since the cross-section for neutron capture is the highest for thermal neutrons, to reach deeper tumours, epithermal neutrons are used and thermalised within the patient. Production of the epithermal neutron beam requires sophisticated moderation assembly, therefore, QA tools to measure the fluence and quality of the beam entering the patient are crucial.

Materials and Methods

We proposed a disposable, miniature Metal-Oxide Semiconductor Field-Effect Transistor (MOSFET) detector with different converters for in-vivo dosimetry of the BNCT epithermal neutron beam components. MOSFET is particularly attractive due to its low voltage or passive operation; the possibility of sensitivity adjustment by biasing the gate during irradiation and/or thickness of the gate oxide (sensitive volume (SV)); the small size of $0.6 \times 0.8 \times 0.35 \text{ mm}^3$; the ability for on-line readout or immediately after irradiation. Two converters were proposed on top of MOSFET- ^{10}B and polyethylene (PE) as well as no converter geometry to measure fluence of thermal/epithermal neutrons, fast neutrons (FN), and γ components, respectively.

Geant4 simulations of the MOSFET response covered with ^{10}B , PE and without converter irradiated with $3 \cdot 10^8 \frac{n}{\text{cm}^2 \cdot \text{s}}$ epithermal neutron beam, in free-air geometry and on the surface of an 18 cm diameter spherical water head phantom were performed for 1-3 μm ^{10}B and 0.2-3 mm PE converter thickness. A one cm diameter spherical target with 40 ppm ^{10}B was placed at 0.5, 1, 1.5 and 2 cm depths in the head phantom. The dose deposited in the SV of the MOSFET and in a 1 cm diameter target was simulated by tracking all secondary particles and their kinetic energy.

Results

The difference in responses between the MOSFET with ^{10}B converter placed on the surface of the phantom and in free air was about 30% due to albedo neutrons. The dose deposited in the SV of the MOSFET with 1 μm ^{10}B converter was much higher than for 1 mm PE converter and should be taken into account when selecting the gate oxide thickness of the MOSFET to provide reasonable sensitivity. Correlation of the MOSFET with 1 μm ^{10}B response placed on the surface of the head phantom and dose in a target will be presented. The thickness of 1 μm ^{10}B and 1 mm PE converters, were found to be optimal for measuring the entrance thermal/epithermal and fast neutron fluence components, respectively.

Conclusion

MOSFET detector with ^{10}B and PE converters can be used to control the epithermal beam quality at the entrance point as a form of in-vivo QA for patients treated with AB-BNCT, and to estimate the dose at different depths within the patient.

Next steps will include simulation of a pixelated 10 cm \times 10 cm 2D transmission detector for real-time monitoring of the 2D flux distribution of the beam components in AB-BNCT.

Abstract ID # 89
Biomedicine &
Food Science

**Klaudiusz
Jakubowski**

First extensive study of lanthanum manganite nanoparticles to target deadly brain cancer

Introduction

The ability to successfully target deep-seated tumours in sensitive areas of the body is limited to adequate targeting strategies. More specifically, brain and central nervous system (CNS) cancers can be the most aggressive, have higher mortality rates and lower accessibility to chemotherapeutic drugs. A proposed solution to target these concerns is through introducing high atomic number (Z) nanoparticles (NPs) such as silver-doped lanthanum manganite (LAGMO) to aid in common treatments such as radiation therapy. These NPs can bypass the blood brain barrier and are capable of increasing the damage from the radiation due to their high-Z. Most importantly they have potential to cause cancer cells to undergo hyperthermia (a cell death precursor) as the NPs heat up in their environment due to their Curie temperature being in the hyperthermia range of interest.

Methods

Magnetic, chemical and biocompatibility characteristics of LAGMO NPs at silver-doping levels of 0-10% were examined. Magnetic and chemical phases of LAGMO NPs were analysed with neutron diffraction using the ECHIDNA High-Resolution Powder Diffractometer. Biocompatibility and combinational treatment strategies involved in vitro biological endpoint clonogenic assays and a cancer cell selectivity investigation.

Results

Neutron diffraction revealed that only 10%-LAGMO NPs exhibit residual ferromagnetism at 300 K compared to other doping levels, suggesting that Curie temperature can be adjusted to the hyperthermia range of interest according to the levels of silver content in the NP. This indicates the potential to induce hyperthermia to cancer cells. Comparative studies on LAGMO NP's biocompatibility with cancer and healthy cells demonstrated healthy cell growth boost and increased cancer cell death suggesting complete cancer cell selectivity. Clonogenic assays also revealed significantly increased cancer cell death with NPs and radiation therapy compared to radiation alone.

Conclusion

LAGMO NPs have immense potential to be used for targeted cancer treatment strategies. They also have the potential to induce cancer cell hyperthermia alongside treatment with radiation due to their magnetic and chemical properties. Furthermore, they have been shown to boost healthy cell growth and severely damage cancer cells alongside radiation."

*Abstract ID # 48
Biomedicine &
Food Science*

Abass Khochaiche

Structural Insights into the Mechanism of Heat-Set Gel Formation of Polyisocyanopeptide Polymers

One of the key factors influencing the mechanical properties of natural and synthetic extracellular matrices (ECM) is how large-scale 3D gel-like structures emerge from the molecular self-assembly of individual polymers. In this talk, I will report the new results on structural characterization of ECM-mimicking polyisocyanopeptide (PIC) hydrogels using small-angle neutron scattering (SANS). The evolution of structure as a function of concentration and background ions across the Hofmeister series will be examined. More specifically, the process of polymer assembly is uncovered by probing the structural features of the heat-set gels and correlating them with their rheological and micromechanical properties. The molecular parameters obtained from SANS show dramatic changes in polymer conformation which map onto the temperature-induced changes in rheological and micro-mechanical behaviour. The formation of larger structures are linked to the formation of cross-links (or chain bundles), whilst the onset of their detection in the SANS is putatively linked to their concentration in the gel. These insights provide support for the 'hot-spot' gelation mechanism of PIC heat-set gels. Finally, it is found that formation of cross-links and heat-set gelling properties can be strongly influenced by ions in accordance with Hofmeister series. In practice, these results have significance since ions are inherently present in high concentration during cell culture studies; this may therefore influence the structure of synthetic ECM networks.

*Abstract ID # 126
Biomedicine &
Food Science*

Gleb Yakubov
Invited Speaker

Chemistry & Crystallography Oral



Atomistic modelling as a complementary tool for diffraction studies

Diffraction experiments typically provide clear picture of a crystal structure and basis for understanding material properties. However, for materials with high static or dynamic disorder and/or weakly occupied atomic sites, the diffraction data reflecting space- and time-averaged state may struggle to distinguish several alternative models yielding similar χ^2 . In that case, atomistic modelling may help not only to identify the more energetically stable configuration but also provide insights into the mechanism of its formation. I will present several recent examples of studies of disordered oxygen and proton ionic conductors, where empirical and ab initio static and geometry optimisation calculations and molecular dynamics simulations not only helped to validate neutron diffraction analysis but also revealed the mechanism driving the disorder.

*Abstract ID # 106
Chemistry &
Crystallography*

Max Avdeev

Hydration mechanisms and lattice distortions in 6H-Ba₄Ta₂O₉

Mixed ionic-electronic conductors have a wide range of applications, including in solid oxide fuel cells, batteries and sensors. Perovskite oxides are well suited for these wide variety of applications due to their robust structures that can be engineered with dopants to achieve desired properties. Hydration, and subsequent oxide-ionic and proton conduction, in such oxides is usually achieved by inserting hydroxide anions into vacancies in the oxide lattice, while the remaining proton from water converts an oxide anion into another hydroxide. We recently used ab initio Density Functional Theory (DFT) dynamics calculations to test the stability of protons and hydroxide ions introduced randomly into a model of the 6H-type perovskite 6H-Ba₄Ta₂O₉. Surprisingly, we found that they robustly and reproducibly combined to form discrete H₂O molecules within an essentially close-packed lattice. Vibrational densities-of-states extracted from the simulations matched well to experimental inelastic neutron scattering data, supporting their validity. The presence of H₂O in 6H-Ba₄Ta₂O₉, vs. hydroxide ions, also explains why it shows substantially lower ionic conductivity than comparable oxides, despite hydrating to a greater extent (0.5 H₂O per formula unit). However, direct crystallographic evidence for the presence of water within 6H-Ba₄Ta₂O₉ at room temperature was lacking. Here, we will present such evidence based on neutron powder and X-ray single-crystal diffraction. We show that water plays a very unusual role in this compound by guiding a unique series of symmetry lowering distortions on cooling, which preserve an otherwise thermodynamically unstable structure to room temperature.

*Abstract ID # 60
Chemistry &
Crystallography*

Chris Ling

Role of A-site molecular ions dynamics in the polar functionality of perovskite metal-organic frameworks

Recent studies on organic-inorganic hybrid perovskites (OIHPs) and ferroelectric metal-organic framework perovskites (MOFPs) reveal their superb performance as highly efficient photovoltaics and promising ferroelectrics. This has enabled a new generation of optic-electronic-mechanical devices based on green chemistry. However, the ultimate strategies to optimize these polarization-related functionalities are not yet clear, leading to confused reports in the literature. In this work, we investigate a rationally selected series of molecular ions within $\text{Mg}(\text{HCOO})_3$ frameworks to form $[\text{CH}_3\text{NH}_3]\text{Mg}(\text{HCOO})_3$ (MAMOF), $[(\text{CH}_3)_2\text{NH}_2]\text{Mg}(\text{HCOO})_3$ (DMAMOF), and $[\text{C}(\text{NH}_2)_3]\text{Mg}(\text{HCOO})_3$ (GUAMOF). Single-crystal X-ray diffraction, inelastic neutron spectroscopy and *ab initio* molecular dynamics are used to achieve detailed structural pictures of three MOFPs. Intriguingly, our study reveals that the alignments of protonated amines are highly dependent on the directional hydrogen bonds that link N-H units to the surrounding MgO_6 octahedra. The alignments of different amines and their dynamics are therefore determined by the acceptor O provided by the distortive frameworks. We successfully assigned the alignments of the A-site ions associated with different polar behavior to the dielectric properties for three MOFPs and propose that the configuration of the A-site molecular ions and potential hydrogen bonds are critical to enable the design of polarization-related functionalities in both MOFPs and OIHPs.

Abstract ID # 13
Chemistry &
Crystallography

Teng Lu

Hydrogen-Bonded Anion Clusters in Choline Phenylalaninate, an Unexpected Origin of Nanostructure in Biocompatible Ionic Liquid

Recently, a number of choline amino-acid salts have been reported to form ionic liquids (ChILs), creating the possibility of biocompatible ILs with a sustainable production cycle.[1,2] Since their discovery, these designer solvents have proven useful across many applications, including drug synthesis and delivery, electrochemistry, biomass processing and CO₂ capture, often in mixtures with water.[3] However, little is still known about how the structure of their constituent ions determines properties and performance of both the pure IL and its solutions, limiting the capacity to design task-specific ILs and optimise for large scale applications. In this study, we investigate choline DL-phenylalaninate (ChPhe) using time-of-flight neutron diffraction and modelled its structure with simulations. Our aim is to understand how its amphiphilic liquid nanostructure arises from atomic correlations. Surprisingly, we discovered the aromatic moieties of the phenylalaninate anion form distinct, small clusters or non-polar domains, but with no evidence for pi-pi stacking. Detailed analysis of the atomic correlations reveals that inter-anion hydrogen bonds are the main stabilisation factor of these non-polar clusters. This is the first example of self-assembled ionic liquid nanostructure not of solvophobic origin. The unusual suite of interactions also explains its water miscibility but inability to retain nanostructure upon water dilution,[4] as well as its poor performance for biomass pretreatment (relative to other nanostructured ChILs),[5] and provides a new strategy by which to engineer and tune ionic liquid nanostructure for the design of application-specific, renewable solvent systems.

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*Abstract ID # 4
Chemistry &
Crystallography*

Shurui Miao

Competitive specific ion effects: A neutron reflectometry study of thermoresponsive polymer brushes in mixed electrolytes

Specific ion effects are phenomena that depend on the identity of ions present in a system, and not merely their valence or concentration. For example, the Hofmeister series orders ions on their ability to either stabilise (salting-in ions) or destabilise (salting-out ions) proteins and is vital in biochemistry.[1] In recent years, polymer brushes, which consist of end-tethered polymer chains to a substrate, have been used as exemplar systems to investigate specific ion effects. [2] The effective solvent quality influences the conformation of these brushes (collapsed or expanded), which is directly linked to application properties (e.g. switchable adhesion and self-cleaning). We have performed a significant body of work on brush conformation in single salt electrolytes.[2-4] However, our understanding of the influence that mixed electrolytes have on the behaviour of polymer brushes is currently limited, which is necessary for real-world applications. Here, we present the behaviour of poly(ethylene glycol) methyl ether methacrylate (POEGMA) brushes in a variety of both pure and mixed electrolytes, as studied with neutron reflectometry. Reflectometry allows for the extraction of volume fraction profiles, which can provide detailed information regarding the influence of ion specificity on polymer brush conformation. Consistent results were also obtained from other techniques, such as ellipsometry, which is used to track overall changes in brush thickness.

In the presence of electrolytes composed of ions from the same end of the Hofmeister series (salting-in and salting-in or salting-out and salting-out), a non-monotonic concentration-dependent influence of the two ions was observed. The specific ion effects imparted by two salting-in ions were dependent on the influence of the ions with the polymer chains. In contrast, the impact of two salting-out ions was dependent on the available solvent molecules. In the presence of electrolytes composed of ions from opposite ends of the Hofmeister series (salting-in and salting-out), ion behaviour was observed to be temperature-dependent.[3] Much can be gained by improving our knowledge of ion specificity and understanding the subtle structural changes of a brush are essential in order to unravel the dominant drivers behind specific ion effects.

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*Abstract ID # 62
Chemistry &
Crystallography*

Hayden Robertson

The scheelites are a family of compounds with chemical formula AB₂O₆ where A and B can represent a variety of different cations. The highly versatile scheelite crystal structure consists of A O₆ octahedra and B O₄ tetrahedra and gives rise to a variety of interesting properties depending on the combination of cations.¹ Scheelite-type oxides including CaWO₄, BiVO₄ and NaLa(MoO₄)₂ have been extensively studied for applications exploiting some of these properties including luminescence, ferroelectricity, ionic conductivity and photocatalytic activity. In particular, Bi³⁺ containing molybdates are efficient photocatalysts^{2, 3} due to the strong repulsive force of the 6s² lone pair of Bi³⁺, resulting in distortion of the B O₄ tetrahedra and alteration of the band gap.

The compound of interest in the present study, Bi₃FeMo₂O₁₂ (BFMO), was reported by Sleight et al. in 1974 as the first scheelite-type compound containing trivalent cations on the tetrahedral site.⁴ Notably, two different polymorphs of BFMO can be isolated.⁵ The ideal tetragonal scheelite-type structure in space group I 4₁/a (#88) can be prepared by a wet chemical route from aqueous solution of the constituent elements. Jeitschko et al. reported in 1975 that, when the tetragonal scheelite structure is heated above 600 °C for ~10 h, a 2:1 ordering of the Mo and Fe cations occurs, which lowers the symmetry to monoclinic in space group C 2/c (#15), and gives rise to a tripling of the a axis.

Here, phase pure BFMO in the disordered tetragonal structure was synthesized by a wet chemical route. The conversion from the disordered tetragonal to the ordered monoclinic structure was examined by in situ neutron powder diffraction in order to understand the temperature dependence of the phase transition and cation order in the mixed metal bismuth scheelite. The study shows no amorphization prior to the formation of the ordered monoclinic phase. Given the substantial cation movement involved in such a transformation, the lack of structural break-down suggests that a certain degree of local cation order may already exist in the tetragonal phase, facilitating the conversion into a fully ordered monoclinic structure. This hypothesis is further supported by an opening in the field-dependent magnetization curve of the tetragonal phase at 1.8 K.

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*Abstract ID # 55
Chemistry &
Crystallography*

**Matilde
Saura-Múzquiz**

Cultural Heritage

Oral



Neutron Imaging: benefits and Case Studies in Palaeontology and Cultural Heritage

Conventional and synchrotron-based X-ray computed tomography (XCT) have been utilised for many years as critical tools in uncovering 3-D internal and surface renderings of scientifically important fossils, cultural artefacts and other specimens held in museum and university collections. DINGO, Australia's thermal-neutron micro-computed tomography (nCT) instrument, is being used to obtain unprecedented renderings of extraordinary fossilised anatomical features not visible with conventional imaging techniques, and yielding new insights into ancient manufacturing methods of archaeological artefacts not attainable by other methods.

NCT is a complementary tool to XCT, and it is important to recognise the benefits, and challenges with its application. Using a selection of case studies from our instrument user program, this presentation will illustrate how neutrons are revealing soft-tissue remains in Jurassic stem-mammals, being used to identify touch-ups and fraud in palaeontology, and providing new insights into Cretaceous polar ecosystems. Through the ANSTO supported Cultural Heritage project, neutron imaging is being used to reveal ancient weapons manufacturing practices, reveal hidden texts in a lead scroll and identify the recycling of mummified votive offerings in ancient Egypt. Improvements in imaging technology and methods at ANSTO is enabling us to achieve higher throughput of these precious objects, minimise neutron-induced activation of samples and to support an increasing number and diversity of student-led research projects.

*Abstract ID # 90
Cultural Heritage*

Joseph Bevitt

Residual stress measurements for cultural heritage

The neutron residual stress analysis can be used as a forensic method for studying non-destructively objects of cultural heritage. A number of case studies on ancient weaponry were collected over the period of the Cultural Heritage Project at ACNS, ranging from the bronze age blades to more recent iron age swords. In the given presentation, the use of the neutron diffraction method is illustrated with these case studies together with the interpretation of the results of stress measurements.

*Abstract ID # 104
Cultural Heritage*

Vladimir Luzin

The application of science and technology to the characterization and the conservation of heritage materials has significantly increased over the last decades. Due to the manifold nature and the value of artefact of cultural heritage significance, studies in archaeometry require a transdisciplinary approach as well as the use of non-invasive multiple analytical techniques.

Today ANSTO's large suite of capabilities and expertise is available for cultural heritage research. In order to promote access by cultural institution and researchers to the unique range of nuclear methods available across ANSTO's campuses, a strategic scientific research project on Cultural Heritage was initiated in 2015.

This paper will showcase how neutron methods have been successfully applied in a series of forensic investigations conducted in close collaboration with Australian and international museums, institutions and universities.

*Abstract ID # 124
Cultural Heritage*

Filomena Salvemini
Invited Speaker

Earth & Environment Oral



Hydrated forms of cryosalts in frozen brines play important roles in the polar landscape and troposphere of Earth [1], and their melting [2] is implicated in recurring slope lineae (RSL) in Antarctica's McMurdo Dry Valley [3] and equator-facing, mid-latitude (42°N-52°S) slopes of Mars [4]. Observation of the widespread occurrence of clay minerals and salts on the Martian surface [5] indicates that saline groundwater [6] may still be present on Mars. The surface of Mars ranges in temperature from 293 K on the equator at noon to 120 K at the poles and mobility of sub-surface water ice will depend on the local temperature and the mobility of confined water in the crustal clays.

We applied quasielastic neutron scattering using the backscattering spectrometer EMU (Australian Nuclear Science and Technology Organisation) at 1 μ eV resolution, to the system: sodium montmorillonite – 5M NaCl (Na-Mt-NaCl) and calcium montmorillonite – 5M CaCl₂ (Ca-Mt-CaCl₂); to establish boundary conditions influencing the dynamics of confined water. Results from elastic fixed window (EFW) data indicate a substantial increase in the mean square displacement of hydrogen (H) in the brine conditions at all temperatures above 100K, indicating enhanced mobility of water in the presence of brines. A phase transition was observed in Na-Mt-NaCl at 255K (on heating) indicating the presence of the cryosalt hydrohalite (NaCl·2H₂O), but no phase transition was observed in Ca-Mt-CaCl₂. In addition, quasielastic neutron scattering (QENS) spectra highlighted that water in the Ca-Mt-CaCl₂ system was strongly confined at room temperature. Recently [6] hydrohalite was observed to form in frozen gels of Na-Mt brines, but not in Ca-Mt brines. They considered that textural differences in the two forms allowed the gel pores of the Na-Mt to retain liquid saline pore water to well below the freezing point of pure water. Based on our analysis, water is restricted to rotational mobility in the Na-Mt-NaCl below 255K, but presents more translational mobility above 255K. These findings largely support those of Yesilbas [7] in the importance of pore structure in controlling cryosalt formation, and further implicate their role in associated phenomena such as RSL.

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Abstract ID # 3
Earth & Environment

Will Gates

Water was discovered 1.5 km below the surface of Mars in 2018 and some liquid water may occur transiently on the Martian surface in the spectrally dominant phyllosilicate group, smectite. In the same year, NASA confirmed that water ice is present in silicates on the surface of the Moon in the polar regions. This discovery has prompted the return of people to the Moon, whereby the Artemis program planned for 2024 will see the next man and the first woman land at the South Pole. The extraction of trapped and frozen water from minerals on other planetary bodies such as the Moon and Mars is a technical challenge if humanity is to implement an innovative and sustainable program of exploration enabling human expansion across the solar system.

We have investigated the hydration properties of clays and minerals found on Mars using time-of-flight neutron spectroscopy. [1] From Quasi-Elastic Neutron Scattering data we determined water diffusion coefficients for input into our model to identify possible sites where the water resides in Na-smectites. Additional characterisation of montmorillonite has been conducted at the Australian Synchrotron facility using far-infrared radiation to obtain proportions of bound and unbound water in Na- and Ca-smectite. We observed the cation rattle at low energy ($\sim 45 \text{ cm}^{-1}$) as a distinct signal from that of the bulk-like water and cationic bound water, where the latter is 'trapped' within the clay layers. [2,3]

Understanding of water hydration processes in these abundant soils and minerals will be of use not just on other planetary bodies but also in extreme environments such as Antarctica. On Earth, knowledge of water dynamics at clay mineral surfaces can be utilised to improve performance and durability of lining materials for barriers used in environmental protection. [4]

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*Abstract ID # 95
Earth & Environment*

Gail Iles
Invited Speaker

Tracking the diffusion of hydrogen rich liquids in shale rocks

Understanding flow of hydrogen rich liquids in shale rocks is critical for the recovery of unconventional hydrocarbon resources. The most common hydrogen rich liquids pertaining to shale rocks are water and oil. The extensive research on water and oil flow in shale rocks has not yet been able to explain the significant uncertainties and discrepancies in reported experimental data. Specifically, what has perplexed the research community is that despite oil spreading more than water on shale surfaces in an inviscid medium, its uptake by shale pores under pure capillary forces is much less than water contrary to theoretical expectations. This causes misjudgement of shale wettability and the underlying physical phenomena.

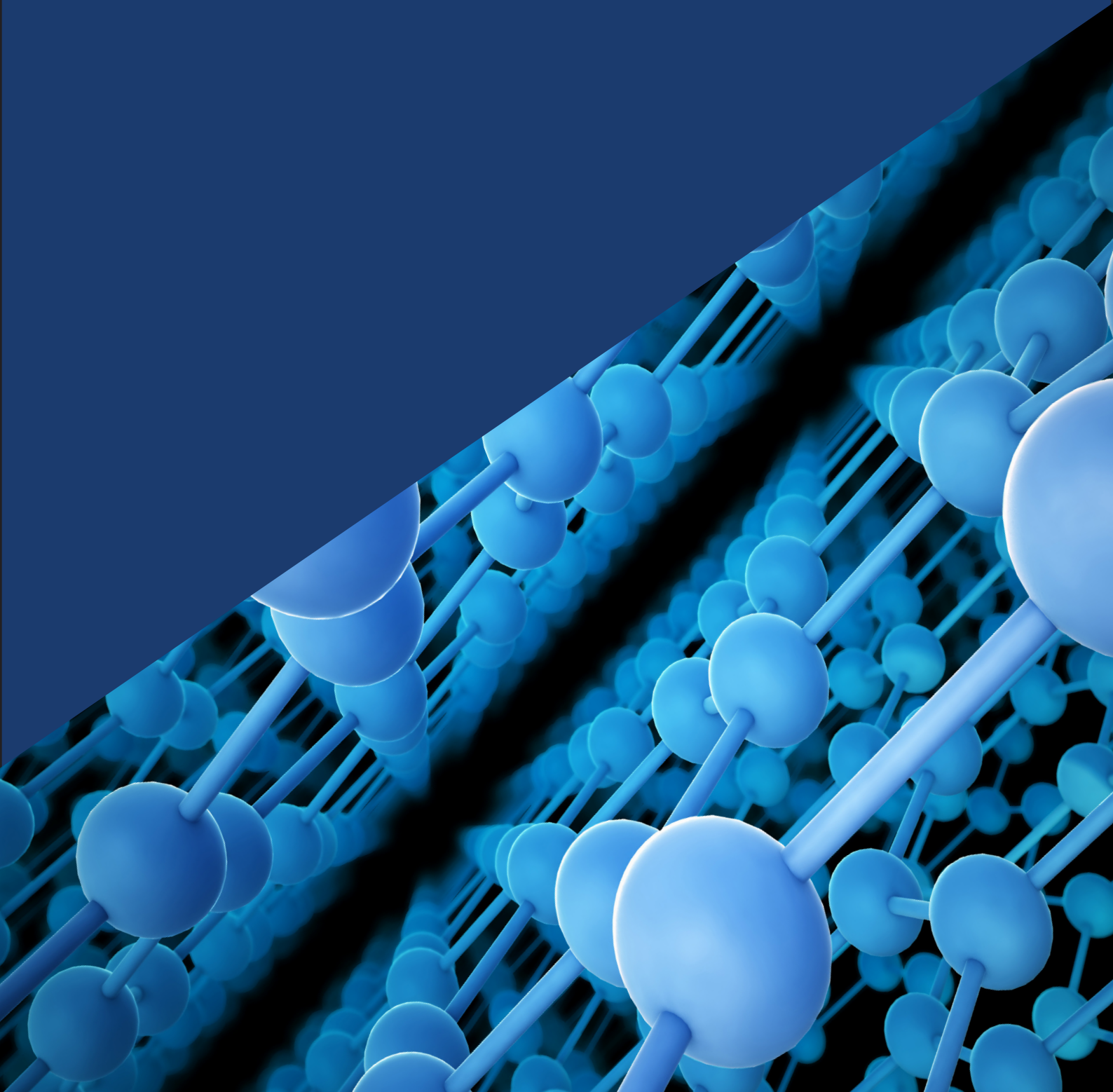
Therefore, in this study, we have used neutron computed tomography (CT) in combination with other experimental and digital rock methods to investigate water and oil flow in an organic-rich shale from the Beetaloo sub-basin in Northern Territory, Australia. The experimental techniques included, in addition to neutron CT, contact angle and spontaneous imbibition tests, X-ray CT, and small angle X-ray scattering. We also used non-equilibrium thermodynamics to theoretically derive constitutive equations to support our experimental observations of configurational diffusion.

The results of this study indicated that the pre-existing fractures imbibe more oil than water consistent with theory. However, theoretically in contrast, the overall imbibition was higher for water than oil. The reason for this was revealed by neutron CT to be greater water diffusion into the shale matrix (second continuum) from the fractures. It was shown that more water uptake into shale was controlled by pore size and accessibility in addition to capillary or osmotic forces i.e. the diffusion type is configurational where water molecules have easier access to smaller pores due to their smaller molecular size compared to larger oil molecules. Thus, even the inorganic pores which seem more oil-wet in an inviscid medium, easily allow water molecules to pass through them compared to oil. On the other hand, strongly oil-wet pores possessing strong capillarity cannot even imbibe oil simply due to its large molecular size and physical inaccessibility to the micro-pores. A combination of neutron and x-ray CT methods revealed that different flow mechanisms are dominant in different continua of shale rocks- and that these mechanisms are dependent on the relative sizes of liquid molecules and pores. The results provide new insights into the previously unexplained discrepancy regarding water and oil uptake capacity of shale rocks.

*Abstract ID # 28
Earth & Environment*

Mohammed Siddiqui

Magnetism & Condensed Matter Oral



Comparing inelastic neutron scattering with theory to understand the complex magnetic interactions in a low-dimensional frustrated magnet

Frustrated magnetic systems have gained a lot of recent interest as they can exhibit exotic magnetic quantum states such as spin-liquid and spin-nematic states [1,2]. The natural mineral atacamite, $\text{Cu}_2\text{Cl}(\text{OH})_3$, is one such material which has been reported to exhibit magnetic behaviour characteristic of a frustrated quantum magnet [3]. It also shares structural similarity with another cuprate, herbertsmithite, whose kagomé lattice is predicted to host a spin liquid ground state [4].

Little is understood about the magnetic properties of the natural orthorhombic structure of atacamite in contrast to its other structural polymorphs. This work studies this lesser understood orthorhombic atacamite, where Cu^{2+} ions form a pyrochlore lattice. The novel magnetic interactions and quantum states in materials like atacamite lends itself to spintronic applications where understanding spin interactions can unveil opportunities for intentionally manipulating these spins.

Time-of-flight inelastic neutron scattering measurements on single crystalline atacamite have been performed at Pelican with an incident wavelength of 4.69\AA . Excitations were observed at 1.5K , and weakened as temperature was increased beyond the antiferromagnetic transition temperature of $T_N = 9.0\text{K}$ [5] to 20K . The strongest dispersion was found along the $H00$ direction with two nested modes observed up to an energy transfer of 3meV . Relatively weak dispersion was seen along $00L$, and a flat mode was observed in out-of-plane scattering covering a narrow section in $0K0$.

Ab initio band structure calculations have indicated a 1D sawtooth chain model for the dominant magnetic exchange paths in atacamite [6]. This chain model can be consolidated with our neutron scattering measurements and SpinW calculations. However, the relative magnitudes and directions of the predicted exchange couplings indicate the strongest interactions to be along $0K0$, and this does not agree with the strongest dispersion measured experimentally in the $H00$ direction at zero field.

To better understand the interactions in atacamite, in-field time-of-flight measurements have also been conducted in magnetic fields up to 6.5T , applied along the crystallographic b -axis. Data were collected using Pelican and the new open geometry, fully compensated, 7T vertical magnet.

We will present the results of these inelastic neutron scattering measurements along with corresponding SpinW calculations to address the inconsistencies between theory and data when considering the exchange interactions in atacamite.

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*Abstract ID # 66
Magnetism &
Condensed Matter*

Jackson Allen

Sub-3nm cobalt nanoparticles embedded in titania glass via ion implantation studied by polarised neutron reflectometry

Synthesis of stable metallic cobalt particles at the nanoscale is challenging using chemical methods due to their unstable nature and their tendency to oxidise. Nevertheless, ultra-small metallic cobalt nanoparticles offer unusual electronic and magnetic properties including large spin moments and magnetic anisotropy[1] [2]. Here we report the use of ion beam implantation to synthesis stable metallic cobalt nanoparticles embedded within TiO₂-x thin films. Scanning transmission electron microscopy (STEM) images revealed that the Co nanoclusters were around 1-3 nm in size. The blocking temperature of Co nanoparticles is estimated to be $T_B = 6.5$ K from the field-cooled and zero-field-cooled magnetization curves. Polarised neutron reflectometry (PNR) measurements reveal superparamagnetic behaviour with a strong temperature dependency due to the small size of the nanoclusters. The nuclear scattering length density, together with near-edge X-ray absorption spectroscopy (NEXAFS) show that the magnetic cobalt clusters are metallic and unoxidized below the TiO₂-x surface, whereas near the surface the clusters are prone to form cobalt oxides in a magnetic dead layer that extends over a few nanometers. Our results show that ion beam synthesis can produce ultra-small particles that are not possible with other methods, and these particles survive for long periods without much oxidation.

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Abstract ID # 118
Magnetism &
Condensed Matter

Abuduliken Bake

Inelastic Neutron Scattering of Lanthanoid-Radical Molecular Nanomagnets

Single-molecule magnets (SMMs) are materials which exhibit slow relaxation of magnetization and quantum tunneling of molecular origin. These properties make them promising for future applications in high-density data storage, as qubits in quantum computing, and in molecular spintronics.[1] The best performing SMMs are complexes of the late trivalent lanthanoid (Ln(III)) ions. The energy barrier to reversal of magnetization here stems from the crystal field (CF) splitting of the spin-orbit coupled ground state with total angular momentum J . The identity and geometry of the coordinated ligands determines the relative order, energy and composition of these CF states, such that appropriate choice of ligands can tune the CF splitting and therefore the SMM behaviour.

Incorporation of organic radicals can be used to improve SMM behaviour, by shifting quantum tunneling of the magnetisation, a through-barrier relaxation pathway, from zero field.[2] The nature of magnetic exchange coupling between a Ln(III) ion and another paramagnetic moiety is, however, hard to determine, and often cannot be determined directly due to the large spin-orbit coupling inherent in many Ln compounds. Inelastic neutron scattering is a powerful experimental technique for directly measuring the CF splitting and exchange coupling in Ln(III) compounds.[3]

Our group has been studying a family of compounds with formula $[\text{Ln}(\text{dbsq})\text{Tp}_2]$, $\text{Tp}^- = \text{tris}(\text{pyrazolyl})\text{borate}$, $\text{dbsq}^- = 3,5\text{-di-tert-butyl-semiquinonate}$, which show exchange coupling between the Ln(III) ion and the dbsq organic radical.[4] We have studied the INS spectra the Ln = Tb, Ho, Er, and Yb analogues on the cold neutron time-of-flight spectrometer PELICAN, as well as their magnetic properties. We observe temperature dependent CF transitions, which are compared to the energy level splitting obtained from electronic structure calculations, as well as exchange transitions in two analogues, which give us both the magnitude of and spatial information about the exchange coupling in this family of compounds.

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Abstract ID # 83
Magnetism &
Condensed Matter

Maja Dunstan

Neutron scattering study on materials with colossal barocaloric effects

Caloric materials are systems that exhibit significant thermal effects at phase transitions induced by external fields like temperature, pressure, stress, magnetic fields, and so forth. They can be used for the solid-state refrigeration through a designated cooling cycle. The core physical issue of caloric materials is the evolutions of atomic structures and interactions as a function of these driving forces in multiple spatial and temporal scales. State-of-the-art characterization techniques based on large-scale facilities such as neutron scattering are highly desirable in this case due to the powerful experimental abilities and versatile sample environments. In this presentation, I will report several case studies of colossal barocaloric effects using neutron scattering techniques. Pressure-dependent neutron scattering measurements on the prototype neopentylglycol as well as other novel systems reveal that colossal barocaloric effects can be attributed to the interplay between extensive orientational disorder and anharmonic lattice dynamics of materials.

*Abstract ID # 17
Magnetism &
Condensed Matter*

Bing Li
Invited Speaker

Infrared catastrophe in two-dimensional quantum antiferromagnets: spectral damping without quasiparticle decay.

We consider two-dimensional quantum antiferromagnets in disordered phases. The disorder can be due to a finite temperature or due to the quantum Lifshitz criticality. In these situations quasiparticles have very long or even infinite lifetime. We demonstrate that in spite of very long lifetime of quasiparticles such systems manifest a broad non-Lorentzian frequency response to a physical probe. This analysis forms the basis for a new paradigm describing the interaction of experimental probes with a physical system, where broadening is due neither to the lifetime, nor to the emergence of fractional quasiparticles. Instead, strong fluctuations drive the probe to absorb and radiate an infinite number of arbitrarily low energy quasiparticles, leading us to draw parallels with the infrared catastrophe in quantum electrodynamics.

*Abstract ID # 65
Magnetism &
Condensed Matter*

Oleg Sushkov

Manufacturing & Engineering Oral



'One layer at a time': Unlocking Novel Materials and Structures for Neutron Radiation Environments through Additive Manufacturing

The fact that neutrons can penetrate deeply makes them an excellent tool for probing the inner structures of materials, however this property also means that effective management of neutron radiation is a central challenge in nuclear engineering, neutron beam science and in the electronics industry. Neutrons also form a significant proportion of space radiation, and therefore novel, lightweight materials and structures for space radiation shielding are at the forefront of Australian and international space science development. Additive Manufacturing provides opportunities for creating novel structures with often complex geometries – and in materials not otherwise possible with traditional manufacturing techniques.

We have brought together a team through the ANSTO-UOW Seed Funding Scheme to focus on the question: “Can the structures and materials made possible by additive manufacturing enable novel solutions for neutron radiation environments?”

Our work to date has focused on three main themes:

THEME 1 – Polymers for neutron shielding and collimation: particularly focusing on boron nitride/polymer composites and the possibilities these composites, coupled with 3D printing techniques, can open for neutron shielding and collimation applications – both terrestrial- and space-based

THEME 2 – Low-hydrogen polymers for neutron sample environments: focusing on 3D-printable polymers for additive manufacturing low-background components for neutron sample environments

THEME 3 – Metals and alloys for neutron sample environments: investigating additive manufacturing of metals – particularly aluminium – and alloys for neutron environment components. This presentation discusses the opportunities and some of the promising approaches for neutron environment additive manufacturing and novel composite materials – with specific examples and initial results from this collaborative endeavour.

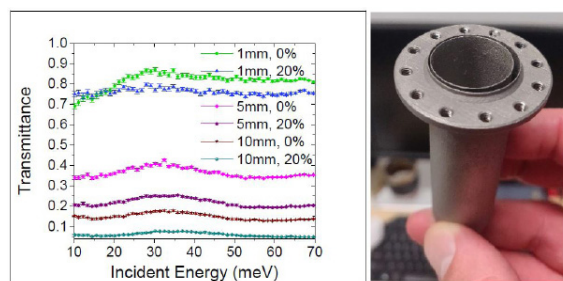


Figure 1 - Neutron transmission reduction from different thickness/BN % configurations of boron nitride/polyurethane composite samples - taken at ANSTO using the Taipan instrument (left); and titanium 3D printed 'sample can' geometry (right) showing the capabilities of metal additive manufacturing for producing neutron environment components.

Abstract ID # 127
Manufacturing &
Engineering

Jonathan Knott
Invited Speaker

Current high-pressure capabilities at ACNS and future plans

High-pressure (>1 Kbar) is a marvellous variable, which can reveal mechanical properties, structural transitions and exotic behaviours. This pairs very well with neutron scattering, where the highly penetrating nature of neutron beams is ideal for accessing sample within complex sample environments. The Australian Centre for Neutron Scattering (ACNS) has developed a number of capabilities for high-pressure experiments, mainly revolving around the use of our Paris-Edinburgh press but more recently with miniature diamond-anvil cells. Some of these, such as our ability to compress radioactive samples as well as combining high-pressure and high-electric fields are unique in the world. Here we review the high pressure capabilities at ACNS, and outline some directions for capabilities and measurements.

*Abstract ID # 35
Manufacturing &
Engineering*

**Helen
Maynard-Casely**

The effects of Bi addition on the mechanical properties of eutectic Sn-Ag-Cu lead-free solder alloy

Sn-Ag-Cu (SAC) solders are gaining momentum as the choice of Pb free electrical interconnect materials because of the legislative restrictions on the use of hazardous materials in electronic devices. However, SAC has high melting temperatures around 217°C. The role of Bi substitution to lowering solder joint processing temperatures are widely considered because of the low-temperature Sn-Bi eutectic. However, the embrittling effects of Bi addition require clarification on the maximum limits of substitution. In this work, the mechanical properties of eutectic SAC with gradual Bi substitution up to 10wt.% Bi was followed. It is shown that fracture strength (σ_f) increases from 50MPa plateauing at 60MPa between 1.4 and 1.8%Bi representing the limits of solid solution strengthening. Over this substitution range, strain at fracture (ϵ_f) dropped from 30% to 10% and reduction in area (RA) dropped from 80% to less than 5%. The σ_f was nearly 80MPa for 2%Bi and this increases gradually with %Bi concentration peaking at 93MPa for 7%Bi. Results of thermal analysis suggested that solidification went off eutectic after Bi concentration exceeded 2%. Using neutron diffraction techniques, the lattice parameter measurements suggest that the solubility limit of Bi in β Sn (in the multicomponent Sn-Ag-Cu) is about 2wt. %. The existence of Bi rich clusters was responsible for observed brittleness after 2wt.% Bi substitution. With the aid small angle neutron Scattering (SANS) and ultra-small angle neutron scattering (USANS), it was found that the intensity changes with respect to scattering factor (Q) especially for high Q region when the precipitations sizes are below 12.5 nm after concentration exceeded 2%Bi that confirms the existence of primary nanosized Bi precipitates that starts to grow into well-defined Bi phases for higher Bi content.

Abstract ID # 112
Manufacturing &
Engineering

Ayodele Olofinjana

Thermal and Mechanical Analyses of Dental Composites for Class II Cavity Restoration in a Molar Tooth: A Finite Element Study

Flowable dental resin composites have substituted mercury-based amalgam as dental restorations over the past decade due to amalgam's biological adverse effect. The flowable dental resin composites are more preferred due to their material properties, aesthetics, and minimal invasiveness. Therefore, the effect of thermal and mechanical stimuli on resin dental composites is an area of active research. This study describes the construction of three-dimensional finite element models of a posterior molar tooth based on data obtained from micro-CT. The scanned tooth consisted of 872 slices that were segmented and meshed in Mimics Innovation Suite software to obtain separate geometric models of enamel, dentine, and pulp. The segmentation process involved mask creation through threshold sets, followed by manual inputs through multiple slice editing. Geometric models were imported to a commercial finite element analysis (FEA) software and conditions such as an intact, cavitated, and filled tooth were simulated for Class II dental cavity restoration. The material properties of each model were assumed to be homogenous and isotropic with elastic behaviour. Transient thermal analysis was conducted to determine the temperature change within each model. The ambient tooth temperature was assumed to be 37°C with extremities in thermal stimuli to be 2°C and 50°C. Moreover, the models were subjected to loading of 400N on the occlusal surface to imitate a bite force at ambient tooth temperature. The strain and stress distributions in the tooth, and tooth restoration, due to thermal and mechanical loading, were studied to optimise the Class II dental cavity restoration. The finite element simulations showed that restorative filling materials with higher Young's modulus and larger coefficient of thermal expansion independently results in higher stress levels. The regions of higher stress on the tooth model were detected and the effects of temperature and mechanical load variations on restoration microleakage were discussed. This study investigated the potential application of three-dimensional finite element modelling for optimizing restorative materials.

Keywords: Dental composite; Thermal stress; Temperature distribution; Strain analysis; Finite element method; amalgam; Flowable.

*Abstract ID # 86
Manufacturing &
Engineering*

**Jerrin
Thadathil Varghese**

Austenite formation kinetics from multicomponent cementite-ferrite aggregates by in situ neutron powder diffraction

The development of third generation advanced high strength steels (AHSS) as the next generation sheet steel grade is driven by the automotive industry. The key processing step is called 'intercritical annealing' at temperatures in the region of the ferrite and austenite two-phase field. The transformed austenite during intercritical annealing will be retained at a metastable state in the final microstructure. Controlling the fraction and chemistry of austenite and resulting mechanical properties is critical for many AHSS.

The kinetics of austenite formation depend sensitively on the initial microstructure and annealing conditions. In this talk, we will present detailed kinetic studies of austenite formation from cementite-ferrite aggregate in a range of AHSS grades via in situ neutron powder diffraction at WOMBAT. The quantitative phase analyses highlight that the saturation of transformation kinetics in relation to global equilibrium is affected by the competition between different interface migration. Depending on the relative contribution of cementite dissolution in respect to migrating interface of austenite/ferrite, the incomplete dissolution of enveloped cementite limited by slow diffusion in austenite could result in austenite plateauing below equilibrium, while fast dissolution of matrix cementite could result in austenite plateau above equilibrium. Both contributions need to be considered and modelled to describe the austenite formation kinetics. The experimental and computational work in this contribution would guide future processing and alloy design of AHSS.

*Abstract ID # 91
Manufacturing &
Engineering*

Yuxiang Wu

Neutron Instruments & Techniques

Oral



ACNS Sample Environment Update

The sample environment suite at ACNS has continued to grow. In the last year we have successfully commissioned our new helium dilution cryostat and the 7T magnet. The magnet has brought important capability for experiments requiring magnetic field to Pelican. We will talk about these new capabilities, how to get the best out of our suite of equipment and some recent unique and interesting sample environment set ups. We will also launch our handbook, covering everything you need to know about our equipment.

We have a number of exciting projects coming up to show you. We are currently working on Direct Laser Melting (DLM) deposition system co-funded by a NSW RAAP grant. Also underway are LIEF grants with equipment for use at ACNS, one includes a rheometer for use on ACNS beam instruments.

In the middle of 2021 we will receive funding to replace our older equipment. The NCRIS RIIP scheme will fund new cryofurnaces, a new type of furnace, a uniaxial press and other equipment.

*Abstract ID # 61
Neutron Instruments &
Techniques*

Tim D'Adam

Potential spectrometers for the hot neutron source at ACNS

The ACNS has a number of spectrometers that are successfully operated in the cold and thermal neutron regime. Interestingly the OPAL reactor is also designed with a position available for a hot source in the reflector vessel, and with two beam-ports available, HB1 and HB2, to deliver hot neutrons. A wide range of studies that will be achievable due to the larger range covered in Q - ω space if the hot source is built are highlighted. These studies range from basic sciences, involving magnetism and superconductivity, crystal fields, molecular studies, high pressure studies etc., to applied work involving, for example, energy and electronic materials, and catalytic processes. An energy transfer range from 5 meV to 500 meV and above, and a momentum transfer range from 0.5 $1/\text{\AA}$ to 30 $1/\text{\AA}$ is indeed possible given the type of instrument designed. Here two types of filter spectrometers are discussed as potential candidates along with a novel type of time of flight spectrometer design that may allow fluxes to be obtained comparable to similar spectrometers on spallation neutron sources.

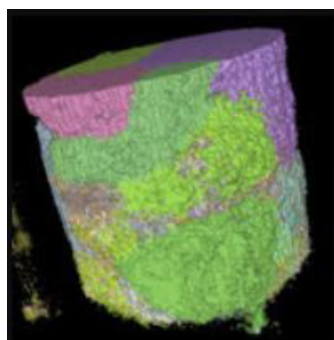
*Abstract ID # 46
Neutron Instruments &
Techniques*

Anton Stampfl

The mechanical and functional properties of polycrystalline materials have significant contributions from the 3D interaction of grains that form their micro-structure. Such grain maps can be extracted from existing characterisation techniques that utilise X-rays or electrons. However, complimentary techniques using neutrons have not yet developed to maturity. Furthermore, neutrons provide distinct advantages where, due to their lower attenuation, larger materials can be analysed, such as real-world engineering materials.

Here, a novel 3D grain mapping methodology, known as Trindex, has been demonstrated to reveal the micro-structure of a prototypical cylindrical iron material. While there already exist several methods on grain mapping with neutron imaging [1,2], Trindex provides a robust and relatively straightforward approach. Trindex is a pixel-by-pixel neutron time-of-flight reconstruction method which extracts the morphology of grains throughout the sample, in addition to their pseudo-orientations.

Experiments were performed at the SENJU beamline of the Japan Proton Acceleration Research Complex (J-PARC). For the setup, an imaging detector was placed behind the sample with diffraction detectors simultaneously collecting the backscattering from the sample. Such diffraction information will be used to confirm grain orientations. Details of the methodology and the resulting 3D grain maps of materials will be presented.



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*Abstract ID # 59
Neutron Instruments &
Techniques*

Patrick Tung

ANSTO's National Deuteration Facility: Recent advancements and an overview on molecular deuteration capabilities for neutron applications.

The National Deuteration Facility (NDF) at the Australian Nuclear Science and Technology Organisation (ANSTO) provides deuteration through both biological and chemical techniques for a diversity of molecules and applications and is the only facility of its type in the Southern Hemisphere with the specialised expertise and infrastructure for both biological and chemical molecular deuteration. Molecular deuteration of organic compounds and biomolecules significantly increases the options in complex structure function investigations using neutron scattering and reflectometry, nuclear magnetic resonance (NMR), mass spectrometry (MS) and other techniques. Deuteration (substitution of the naturally occurring hydrogen stable isotope deuterium (^2H or D) for ^1H (or H)) can provide contrast and improved resolution to assist investigations into the relationship between molecular structure and function of molecules of both biological and synthetic origin.

By developing a suite of capabilities in both in vivo deuteration of biomolecules and chemical deuteration of small organic molecules, the NDF provides access to a broad range of deuterated molecules for research and industry. Variably deuterated proteins can be produced via recombinant expression in *Escherichia coli* and other microbial systems utilised to produce deuterated cellulose and cholesterol. By tailoring deuteration approaches with the ongoing development of chemical deuteration protocols for a broader range of molecular classes than available commercially, the NDF has increased the range of systems that can be investigated using deuterated molecules. Lipids, phospholipids (including head or tail or head/tail deuterated mono-unsaturated lipids such as POPC and DOPC), heterocyclics, aromatics, surfactants, ionic liquids, saturated and unsaturated fatty acids, sugars and match-out detergents have been deuterated.

Common neutron applications include partially deuterated proteins for SANS experiments investigating multi-protein systems, neutron crystallography of perdeuterated proteins, neutron reflectometry of lipid bilayers systems and SANS using saturated lipid vesicles, or detergents amongst others.

An overview and update on the NDF will be provided which will include details on the NDF User Program (e.g. information on the available modes of access), recent advancements in custom deuterated molecules available and brief highlights of deuterated molecule utilisation for neutron experiments at ANSTO's Australian Centre for Neutron Scattering (ACNS).

*Abstract ID # 71
Neutron Instruments &
Techniques*

Karyn Wilde

2019 ANBUG Award Winners



Understanding Energy Materials Function: Neutron Diffraction of Materials Not at Equilibrium

The performance of functional materials central to energy devices, including rechargeable batteries, fuel cells, as well as gas separation and storage technologies, is determined largely by atomic-scale materials structure and dynamic-function relations. Many functional materials undergo structural change during use, for example to accommodate compositional change such as in rechargeable battery electrodes that reversibly host charge-carrying ions and in gas storage and separation materials that reversibly host molecular gas species. Robust characterization methods that quantitatively and accurately capture these changes are essential to the strategic design of materials with superior function, and consequently, to improving device performance.

Historically, a conflict existed between fast and detailed neutron scattering measurements of materials, particularly for measurements of materials within devices. This conflict was sometimes alleviated by using small model systems in which the material function was not representative of that in the corresponding commercially-used device. Today, advanced characterization methods that capture material changes in detail while they are occurring is possible in whole devices under real-life operating conditions, as facilitated by advances in instrumentation. This is especially true for powder diffraction, with instruments such as the high intensity neutron powder diffractometer Wombat at the Australian Centre for Neutron Scattering (ACNS) being one of the fastest of its kind globally.

This talk will give examples of real-time neutron scattering measurements of functional energy materials capturing compositional change and non-equilibrium processes, with a focus on neutron powder diffraction using ACNS's Wombat. 1-4

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*Abstract ID # 133
2019 Neutron Award*

Vanessa Peterson

Dynamics in soft matter systems probed by small-angle neutron scattering

Due to the lower intensity of neutron sources when compared to synchrotron X-rays, it is often assumed that small-angle neutron scattering (SANS) is best suited to the study of equilibrium samples or processes with slow dynamics. However, over the last 10 years, my group (and many others) have shown that along with 'slow' processes taking minutes or hours, even fast dynamic processes in soft matter systems can be accessed using neutron scattering. Such measurements provide information on how systems rearrange at the nanoscale, and ultimately, how this informs their bulk properties and behaviour. This talk will explore some interesting cases where dynamic studies using SANS uncover unique properties of self-assembled systems.

Dense microemulsions are particularly suited to study using dynamic SANS 1, as their scattering intensity tends to be rather high. However, this means that analysis of obtained scattering is often compounded by the convolution of form with a strong structure factor contribution from local interactions or structuring between droplets. Dynamics of a dilution-induced phase change between lamellar and droplet-like microemulsion systems could be monitored with time resolution as low as 20 ms, offering new insight into fast processes where the neutron contrast offered by isotopic variation proves essential 1.

Light as an external stimulus to cause dynamic changes in soft matter is particularly appealing, as photons are seen as a 'green' reagent that ideally allow spatiotemporal control of chemical systems. To incorporate this feature into surfactant systems, molecules that photoisomerise are used, termed photosurfactants [2]. By monitoring the changes in self-assembly structure as such systems undergo isomerisation, insight can be obtained on their packing and dynamics, aiding the design of stimulus responsive complex fluids.

Finally, the deformation of self-assembled systems in flow is a fascinating manifestation of the complex interplay between structure and dynamics. Perhaps the most prototypical example of this is how long, threadlike micelles align with a flow field, lowering their entanglement and therefore viscosity. By exploring different shear speeds, information on how structure relates to flow, which is essential in product design using these industry-favourite viscoelastic texture modifiers.

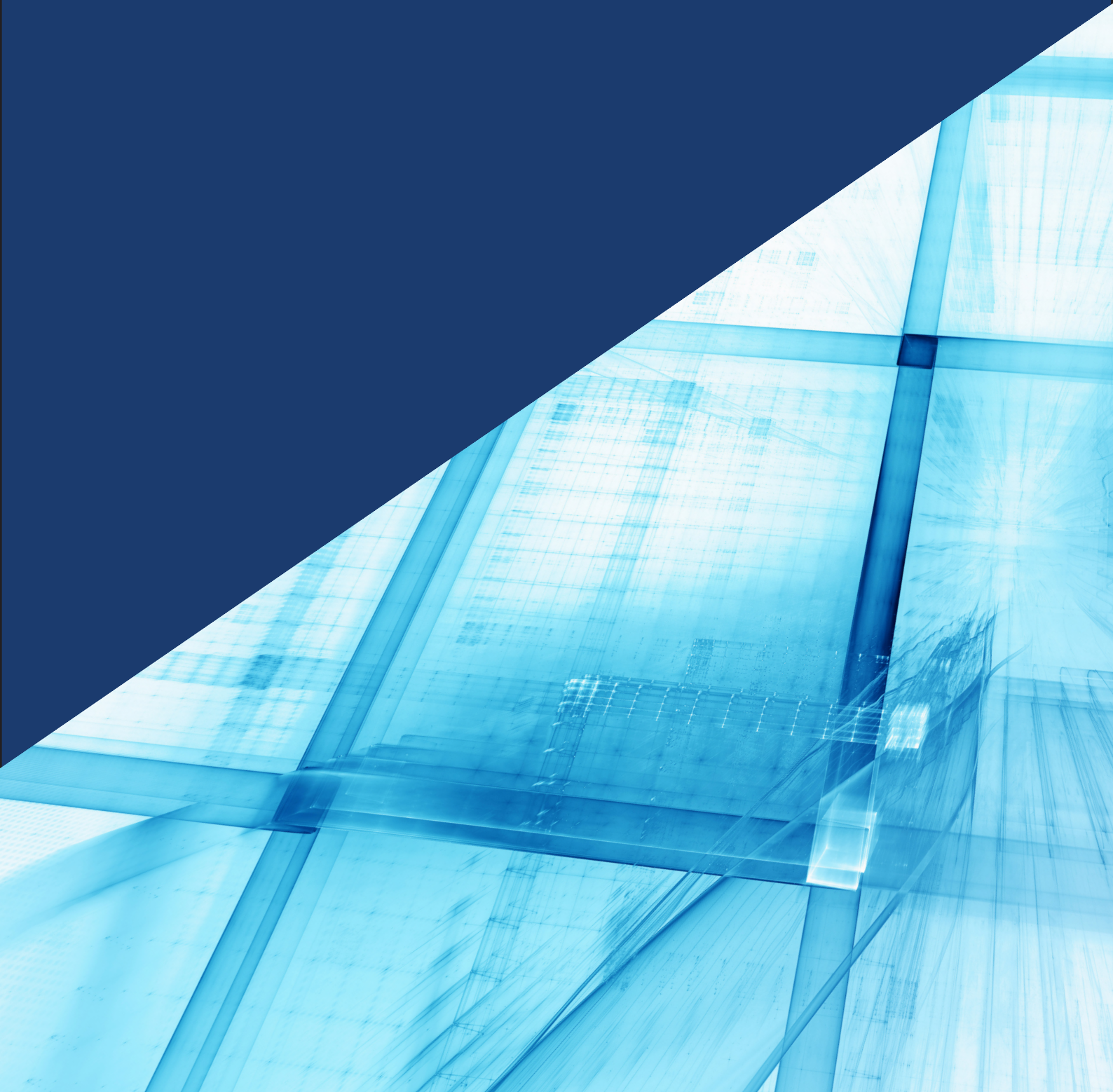
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Abstract ID # 123
2019 Young Scientist

Rico Tabor

Posters



All living organisms rely on membranes that act as selectively permeable barriers controlling movement in and out of cells. Model systems such as tethered-bilayer lipid membranes (tBLMs) can be designed to replicate the fundamental structure and function of their biological counterparts. This creates a simplified pathway for determination of the effects that antimicrobial medicines can have on cell membranes, as well as opening the door for the development of membrane-based biosensors.

The formation of tBLMs involves the binding of tethering amphiphilic lipids to a gold surface to create a monolayer tightly bound through gold-sulphur interactions. Further lipid addition results in a highly stable bilayer design that can be used to mimic bacterial or eukaryotic cell membranes.

The structure of tBLMs and how they change when exposed to antimicrobials and other molecules can be analysed using electrochemical impedance spectroscopy and neutron reflectometry. Resistive and capacitive properties of a model membrane can be approximated with an electrical circuit modelling impedance spectroscopy data, whilst neutron reflectometry provides a layer-by-layer profile of the membrane's core structure.

This work focuses on the use of these techniques to show 1) how pre-treating a model gram-negative bacterial membrane with gold nanoparticles can increase the efficacy of the antibiotic colistin, 2) how model membranes could be used as a more effective screening mechanism for determining efficacy of antimicrobial polymers and 3) how the stability of model membranes can be effected by temporary dehydration through removal of electrolyte solution.

*Abstract ID # 18
Biomedicine & Food
Science*

Alex Ashenden

Status, statistics, and recent research highlights from Echidna

The Echidna high-resolution powder diffractometer remains a reliable and productive ACNS instrument contributing annually to about 50 published studies done on a wide range of topics, from magnetic, energy and planetary materials to cultural heritage and additive manufacturing. We will discuss how Echidna has been affected by COVID-19 measures, latest and planned developments, user programme statistics, and recent research highlights.

*Abstract ID # 53
Biomedicine & Food
Science*

Alex Ashenden

Development of Direct Laser Melting (DLM) deposition system for in-situ use on neutron beam instruments

Direct Laser Melting (DLM) deposition is an additive manufacturing technique in which a high power laser is used to create a melt pool on a workpiece while a jet of metal powder is applied, resulting in localised material deposition. This technique is used in industry for additive repairs, cladding with dissimilar metals, or, in conjunction with a CNC milling machine, as a full-fledged 3D additive fabrication platform. As the prominence of this technology rises, so too does interest in characterising deposition dynamics over a vast parameter space. Neutron beam instruments offer unique capabilities for such characterisation.

As part of the NSW Research Attraction and Acceleration Program, ACNS is developing world first sample environment capabilities enabling in-situ laser metal deposition, for use on KOWARI and DINGO beamline. The system will utilise a self-contained motion stage and laser cladding head which will construct a thin wall structure on a user specified substrate, utilising up to two metal powders at a time. Neutron studies of the melt pool or heat affected zone can then be performed during and after printing.

This paper will present the technical specifications and capabilities of the system, which will be available to the user community in late 2021.

*Abstract ID # 63
Neutron Instruments &
Techniques*

Chris Baldwin

Synthesis-Controlled Polymorphism and Magnetic Properties of $\text{Li}_3\text{Co}_2\text{SbO}_6$

$\text{Li}_3\text{Co}_2\text{SbO}_6$ has been synthesized using high temperature solid-state methods. $\text{Li}_3\text{Co}_2\text{SbO}_6$ is found to adopt two highly distinct structural forms: a pseudohexagonal (monoclinic $C2/m$) layered $\text{O}_3\text{-LiCoO}_2$ type phase with “honeycomb” 2:1 ordering of Co and Sb, and an orthorhombic $Fddd$ phase, isostructural with $\text{Li}_3\text{Co}_2\text{TaO}_6$ but with the addition of significant Li/Co ordering. Pure samples of both phases can be obtained by conventional solid-state synthesis via a precursor route using Li_3SbO_4 and CoO , by controlling particle size, initial lithium excess, and reaction time. Both phases show relatively poor performance as lithium-ion battery cathode materials in their as-made states, but complex and interesting low-temperature magnetic properties.

The monoclinic honeycomb phase is the first of its type to show A-type antiferromagnetic order (ferromagnetic planes, antiferromagnetically coupled), with $T_N = 14$ K. Isothermal magnetisation and in-field neutron diffraction below T_N show clear evidence for a metamagnetic transition at $H \approx 0.7$ T to three-dimensional ferromagnetic order. The orthorhombic phase orders antiferromagnetically below $T_N = 112$ K and then undergoes two more magnetic phase transitions at 80 and 60 K. Neutron diffraction data show that the ground state is incommensurate.

In this presentation the crystal structures of both polymorphs of $\text{Li}_3\text{Co}_2\text{SbO}_6$ will be discussed as elucidated by X-ray powder diffraction and neutron powder diffraction. The low-temperature magnetic ground-states and magnetic behaviour, including in-field metamagnetism displayed by the honeycomb phase will also be discussed.

*Abstract ID # 47
Magnetism &
Condensed Matter*

Alex Brown

Elucidation Of The Wave Function Of The Ground Doublet In A Tb Complex Using INS In A Magnetic Field

Lanthanoid Single Molecule Magnets (SMMs) are molecular materials that exhibit slow relaxation of the magnetisation of molecular origin, thus showing promise for a wide range of technological applications, such as spintronic devices, qubits for quantum computers and molecular memories. The origin of the energy barrier to the reorientation of the magnetic moment in a lanthanoid SMM lies in the weak splitting of the atomic lowest-lying spin-orbit multiplet of the Ln^{III} ion, induced by the electron density of the ligands, into a set of crystal field states. Since the crystal field splitting is significantly weaker than other energy contributions in lanthanoid complexes, the details of the ligand-Ln interaction are crucial for the development of SMMs which can operate at high temperatures.

For this reason, it is crucial to achieve a detailed understanding on how the crystal field influences the relaxation of Ln^{III} SMMs, and to this end computational and theoretical methods have been very useful to rationalise experimental results, and are routinely employed in the molecular magnetism literature. On the other hand, comparison of simulations with different experimental measurements can showcase the shortcomings of the theoretical or computational approach, providing a rationale on the improvements to introduce in order to improve their ability to successfully describe the properties of the system.

Previously, we have performed Inelastic Neutron Scattering (INS) measurements on the complex [Tb(bpy)₂(Cl⁴Cat)(Cl⁴CatH)(MeOH)] using the PELICAN instrument, where we observed a shoulder to the elastic line which, after fitting, was established to arise from a single transition. While theoretical calculations of the low-lying energy spectrum of the complex rationalized the observed transition as arising from the quantum tunnelling of the ground Ising doublet, the predicted tunnelling gap is significantly smaller than what observed experimentally, highlighting the inability of such calculations to correctly predict the electronic properties of the ground state of the molecule.

In this study, therefore, we have measured the INS spectra for the aforementioned complex, under the same experimental conditions of the previous experiment, employing the newly commissioned magnet on PELICAN, where the evolution of the observed transition in an increasing magnetic field would provide useful information on (i) the properties of the ground state and (ii) the nature of the magnetic transition observed in the zero-field spectrum. The measurements show that, with increasing magnetic field, the INS transition (i) becomes less intense, thus confirming our theoretical description of the observed peak as arising from the quantum tunnelling of the ground state, and (ii) splits into multiple peaks, both as a result of the usage of a powder sample and the complex spin-orbit composition of the wave function of the ground Ising doublet.

*Abstract ID # 80
Magnetism &
Condensed Matter*

Simone Calvello

Magnetic Structure and Magnetocaloric Properties of LaMn₂Ge₂

The extensive set of ternary intermetallic RMn₂X₂ compounds (R = rare earth, T = transitional metal, X = Ge or Si) have been investigated extensively in the past few decades due to their interesting range of physical properties [e.g. 1-3]. Recently, significant attention has been paid to the magnetocaloric effect (MCE) of RMn₂X₂ compounds for their potential application in magnetic refrigeration. Their MCE properties are important as RMn₂X₂ compounds enable a wide range of structural and magnetic behaviours and related transitions to be controlled via substitution of R, Mn, and X atoms on the 2a, 4d, and 4e sites respectively [e.g. 4-7].

We have carried out a detailed investigation of the LaMn₂Ge₂ compound using neutron diffraction and magnetic measurements, focusing on the magnetic behaviour of the Mn-sublattice. With decreasing temperature, the magnetic state changes from paramagnetism to incommensurate canted antiferromagnetism AFFs at T_N ~ 360 K and then gives way to incommensurate canted ferromagnetism F_{mi} below T_C ~ 323 K. No obvious magnetoelastic coupling were detected from refinement of the variable neutron diffraction patterns (5 K- 450 K) while detailed analyses of magnetic data indicate that the magnetic phase transition is second order. Under magnetic field changes of 2 T and 8 T, the maximum values of the magnetic entropy change (-ΔE_{ASM} max) around T_C reach 1.65 J/kg K and 4.42 J/kg K, respectively.

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Abstract ID # 81
*Neutron Instruments &
Techniques*

S J Campbell

New insights into colloidal phase transitions using neutron scattering techniques

The fundamentals of crystallisation and glass formation in atomic systems are not yet fully understood. Hard-sphere colloidal nanoparticles have been shown to be promising model systems for understanding crystallisation and glass formation in atomic systems: As colloidal motion is Brownian, rather than ballistic, kinetics and dynamics are orders of magnitude slower than in atomic systems and can be studied in real-time. However, despite previous work, key elements are still missing from our understanding of phase transition in colloidal suspensions especially regarding metastability, supercooling and the glass transition. In particular, there is still no clear understanding of the effects of polydispersity: although studies of both polydisperse and binary mixtures of hard sphere colloids have been performed, a systematic study of the effects of polydispersity on structure, crystallisation kinetics and particle dynamics is still lacking.

One of the reasons for this is the relatively limited types of suspensions which have been studied- most particles used for such studies need to be suspended in mixed solvents for refractive index matching for light scattering studies, which introduces potential problems such as selective solvation and evaporation. In this work we explore the possibility of using ionic liquids (ILs) and deep eutectic solvents (DESs) as the suspending solvent, as these can be tuned to match the refractive index of the particles, and don't suffer from evaporation. We will then develop suitable binary colloidal suspensions consisting of deuterated & non-deuterated nanoparticles suspended in the solvent. With a combination of lab techniques and beam time allocations at the Australian Synchrotron, ANSTO and overseas neutron facilities, we will expansively investigate the nature of metastability, crystallisation and the glass transition, and provide a significant advance on our current understanding of these processes.

*Abstract ID # 100
Chemistry &
Crystallography*

Katherine Chea

Lithium garnet oxides have been put forward as a solid-state alternative for Li-ion electrolytes since the Li⁺ conducting abilities of Li₇La₃M₂O₁₂ (M = Ta, Nb) was discovered in 2003. [1] These solid state materials exhibit physical and chemical properties desired for more efficient and safer Li-ion battery electrolytes. [2] Lithium garnet oxides can exist in tetragonal and cubic phase isomorphs with the latter exhibiting higher conductivities. Li₇La₃Zr₂O₁₂ undergoes a phase transition from cubic to tetragonal due to the thermodynamic unstable nature of the cubic arrangement. [3] Ionic conductivities of up to $1 \times 10^{-3} \text{ S cm}^{-1}$ have been reported for cubic phase garnet materials of Li_{6.4}La₃Zr_{1.4}Ta_{0.6}O₁₂. [4] Here we present a dual doped garnet series of Li_{6.75-3x}Ga_xLa₃Zr_{1.75}Ta_{0.25}O₁₂ and attempt to mimic the high conductivities seen in that Li_{6.4}La₃Zr_{1.4}Ta_{0.6}O₁₂. The successful synthesis of the proposed series was achieved via standard solid-state sintering from gallium doping up to $x = 0.5$. X-ray and neutron powder diffraction characterisation revealed that Ga has a preference to occupy the Li tetrahedral (Li_{24d}) site over the octahedral (Li_{96h}) site. High-temperature neutron diffraction studies show the relationship between temperature, Ga content, and Li displacement between the Li_{24d} and Li_{96h} sites.

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Abstract ID # 49
Chemistry &
Crystallography

Timothy Christopher

Bottom-up fabrication of magnonic crystals utilizing polyoxometalates and block copolymers

Magnonics is a new and emerging field of nanoscale science and technology. The goal of being able to produce magnonic devices is driven by the increasing needs of efficiency and speed of the technological devices our society thrives on. With the increase of energy consumption in the continuously advancing modern age, there needs to be ways in which energy is able to be produced either more sustainably, or the current processes need to be made more efficient. Spin-waves, otherwise known as magnons (hence the term magnonics), are generated when a magnetic disturbance is introduced into a spin-aligned material. This causes the aligned electron spins to precess, which in turn generates a detectable signal. Current data storage sites require a large energy consumption dedicated to cooling, and are often held in low temperature areas like the Arctic circle due to the high amounts of heat that are given off by electronic devices; in theory, magnonics has the potential to minimise the effects of heat since they are low energy systems. To transport magnons in a controlled manner, spin-wave guides are required to direct the signal. Periodically structured magnetic materials are an important aspect in the study of magnonics as the formation of a band gap is required to control the allowed and forbidden magnonic states. It is also important to confine the spin-wave propagation to 2 dimensions in order to minimise the dispersion of the spin-waves once generated. In our research we are looking at using polyoxometalates as the magnetic materials and block copolymers as the structuring agents to fabricate spin-wave guides. Polyoxometalates were chosen as they are a promising candidate for magnonic wave guides, exhibiting structural and magnetic diversity.

In this work, we have used an amphiphilic block copolymer, poly(styrene-block-N-4, methyl vinylpyridine methyl iodide), to encapsulate polyoxometalate clusters in micelles. The highly anionic polyoxometalate species are able to undergo an ionic exchange reaction with the positively charged block of the block copolymer. We have demonstrated that the POMs used can bind to the block copolymer and form uniform micelles that can be deposited as a semi-ordered array onto substrates by spin coating. The resulting materials and films have been characterised at various stages along the way: FT-IR and TGA have shown that the POMs have been successfully incorporated into the polymer and that the amount of POMs incorporated can be controlled. SQUID results have shown that the susceptibility of the POMs is retained once incorporated into the polymer matrix. Dynamic light scattering has been used to find the optimal conditions for micelle formation with respect to both size and polydispersity. Atomic and magnetic force microscopy have shown that spin coating of the micelles onto a substrate forms ordered structuring of the micelles, and that these micelles do in fact show magnetic signals in their cores.

*Abstract ID # 79
Advanced Materials*

Clyde Daniel

Assisting polarized neutron experimentalists: Extracting magnetic depth profiles from ab-initio calculations

The polarised neutron reflectometry (PNR) technique measures the magnetic depth profile with nanometre-scale resolution in thin film structures. Although the raw experimental data can a rich source of qualitative information, to extract the full quantitative details, the experimentalist must solve the inverse-problem by postulating models to fit the data to yield the full set information. In PNR, this can lead to numerous free variables in the model, and unconstrained models are seldom reliable. For solid-state systems, the number of free variables can be greatly reduced by using a variety of complementary techniques including transmission electron microscopy and Rutherford back-scattering to measure the thin film chemical profile, and therefore constrain the nuclear scattering length density of the PNR model. Owing to the unique sensitivity of PNR, however, there are very few complementary experimental probes that can cross-checking the validity of the magnetic aspect of the model. For this reason, our group has developed new approaches using spin polarised DFT calculations to simulate the spin electronic density and perform averaging to mimic the PNR spatial resolution, to compare with experimental data. These ab-initio techniques only require a crystallographic starting model, and full ionic relaxation is performed in large slab models using the GADI supercomputer to reconstruct ultra-thin films (with thicknesses 1-10 nm). For thicker films, our group has explored semi-empirical models based on micromagnetic or Monte Carlo simulations where a model Hamiltonian is simulated.

This poster provide a few demonstrations of these theoretical techniques supporting PNR for studying ion-beam induced effects in exchange-biased effects in Co/Pd hydrogen sensors [1], NiFe/Fe₂O₃ bilayers [2] and FePt₃ alloys [3].

*Abstract ID # 98
Magnetism &
Condensed Matter*

David Cortie

KOOKABURRA, The ultra-small-angle neutron scattering instrument at ANSTO

The double-crystal ultra-small-angle neutron scattering (USANS) diffractometer Kookaburra at ANSTO was made available for user experiments in 2014. Kookaburra allows the characterization of microstructures covering length scales in the range of 0.1–10 μm . Use of the first- and second-order reflections coming off a doubly curved highly oriented mosaic pyrolytic graphite pre-monochromator at a fixed Bragg angle, in conjunction with two interchangeable pairs of Si(111) and Si(311) quintuple-reflection channel-cut crystals, permits operation of the instrument at two individual wavelengths, 4.74 and 2.37 Å. This unique feature among reactor-based USANS instruments allows optimal accommodation of a broad range of samples, both weakly and strongly scattering, in one sample setup [1,2]. The versatility and capabilities of Kookaburra have already resulted in a number of research papers, including studies on hard matter systems like rocks and coal [3,4], as well as soft matter systems like hydrogels, milk or worm-like micelles [5-7]. This clearly demonstrates that this instrument has a major impact in the field of large-scale structure determination. Some of the recent examples will be presented here.

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*Abstract ID # 115
Neutron Instruments &
Techniques*

Liliana de Campo

High-q, High Intensity Small Angle Neutron Scattering to Probe Formaldehyde-Methanol-Water Mixtures

Methanol-water mixtures are known for their unusual thermodynamic behaviour. On varying mixture composition, the thermodynamic properties do not vary linearly. This is attributed to the formation of structures at a molecular length scale, called as micro-phase. When formaldehyde is solvated in methanol-water mixtures, its chemical and physical behaviour is very much dependent on its micro-phase environment. Recently, liquid phase heterogeneous catalytic routes for the production of formaldehyde and its higher order oligomers are being developed^{1,2}. The liquid phase (generally, methanol-water mixture) increases formaldehyde's yield after its desorption from the catalytic surface¹. Therefore, the study of formaldehyde's solvation in methanol-water mixtures may be crucial to further develop these liquid phase catalytic reaction pathways. However, the understanding of the structure of formaldehyde-methanol-water mixtures at molecular length scales is a challenge to the contemporary experimental techniques due to their dynamical and chemical nature. We use molecular dynamics simulations and the Small Angle Neutron Scattering (SANS) measurements to predict the molecular clustering in these mixtures.

Classical Molecular Dynamics (MD) simulations were performed using GROMACS software package³ and the OPLS-AA forcefield parameters were used to describe bonded and non-bonded interactions. The radial pair distribution function $g(r)$ and the coordination number were used to estimate the cluster composition and to compose backgrounds for these ternary mixtures. The Neutron Scattering data was collected at the Quokka beamline of the Australian Nuclear Science and Technology Organisation (ANSTO). The data modelling program SASview was used to model the scattering data and five different curve-fitting models were used, namely, the Guinier model, sphere model, sticky-hardsphere (SHS) sphere model, and SHS ellipsoid model. The sticky-hardsphere model fitting parameters were derived from the Potential of Mean Force (PME), calculated by the MD simulations.

We observe a hydrophobic clustering of methanol around methoxymethanol molecule (i.e., the metastable solvated form of formaldehyde) at formaldehyde-methanol-water mixtures where 1 mole-percent formaldehyde is dissolved in $x_m \leq 0.3$ methanol-water mixture. The SHS-sphere model results in a sphere of 4.29 Å radius, which, when drawn from the centroid of a molecular cluster obtained via MD data, perfectly encapsulates it. On further increasing the methanol concentration, we do not observe any molecular clusters for $x_m > 0.5$. In summary, we formulate a framework of analysing the dynamic ternary liquid mixtures for molecular clustering using SANS measurements and MD simulations and report hydrophobic clustering in formaldehyde-methanol-water ternary mixtures at low methanol composition.

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Abstract ID # 85
Magnetism &
Condensed Matter

Swarit Dwivedi

Diffuse Scattering Studies from a Martensitic Fe-Pd Alloy

From literature reports, Fe-Pd alloys in the vicinity of Fe-30at%Pd exhibit two martensitic transformations on being cooled from just above room temperature to about 100K. A preliminary study of a large single crystal of this composition at the KOALA beamline, not only showed evidence for these transformations but also revealed most interesting satellite reflections around certain Bragg reflections. The crystal has been studied further in two triple-axis experiments. The first was at TAIPAN, specifically to study elastic scattering and the second, at SIKA, to study quasi-elastic scattering both in the vicinity of certain Bragg peaks but also around the satellite reflections observed at KOALA. The results from both of these experiments will be discussed.

*Abstract ID # 22
Magnetism &
Condensed Matter*

Trevor Finlayson

Crystal field interactions in the chiral compounds RNi_3Ga_9 ($\text{R} = \text{Tb}, \text{Dy}, \text{Ho}$ and Er) studied by inelastic neutron scattering

In recent years, compounds with chiral structures have attracted much attention mainly because of noncollinear and non-coplanar spin textures, which have an important application in spintronics. In chiral compounds, the lack of inversion symmetry can give rise to an asymmetric spin interaction, the so-called Dzyaloshinskii-Moriya interaction, which contributes to the symmetric exchange interaction and anisotropy effects from the crystal field. These interactions' coexistence can result in unusual magnetic properties and exotic magnetic structures with potential for many applications and novel phenomena. In this work, we study the magnetic properties of the chiral compounds RNi_3Ga_9 ($\text{R} = \text{Tb}, \text{Dy}, \text{Ho}$ and Er), which crystalize in a trigonal ErNi_3Al_9 -type structure with non-centrosymmetric space group $R\bar{3}2$ [1]. For this purpose, we analyzed the inelastic neutron scattering (INS) spectra in powder samples at several temperatures (T) to study the crystal electric field (CEF) excitations and ground-state. The INS experiments were performed at the SIKA beamline using the cold triple-axis spectrometer. The spectrum was analyzed at four temperatures for ErNi_3Ga_9 ($T = 8, 20, 50$ and 100K) and two temperatures for TbNi_3Ga_9 ($T = 50$ and 100K), HoNi_3Ga_9 ($T = 30$ and 100K) and DyNi_3Ga_9 ($T = 50$ and 100K). Moreover, transverse and longitudinal magnetic susceptibility was measured in single-crystalline samples to fit the CEF parameters better.

We developed a code based on the magnetic susceptibility and differential cross-section for magnetic scattering at low Q (dipole approximation) to process and analyze the experimental data. The effective CEF hamiltonian for the system follows the C_3 point symmetry, which results in 9 CEF parameters overall. The least-square fitting procedure uses a machine-learning algorithm based on particle swarm optimization. We report the energy levels scheme due to the crystal field and the CEF ground state's eigenfunctions. In particular, the INS spectra for the ErNi_3Ga_9 compound showed peaks associated with the so-called hot transitions, which take place between excited energy levels. We only observed peaks associated with transitions between the ground-state and the first excited levels for $\text{R} = \text{Ho}, \text{Tb}$, and Dy . The calculated INS spectra and magnetic susceptibility were in good agreement with the experimental data. In particular, the calculated magnetic susceptibility showed that the direction of easy magnetization occurs along the c -axis for the ErNi_3Ga_9 compound and along the basal plane for the other compounds. It evidences the oblate and prolate nature of the rare-earth ions charge distributions. In summary, we used inelastic neutron scattering data to establish the CEF parameters for all compounds according to the C_3 point symmetry. The obtained parameters describe the CEF energy levels' configuration and the relative intensity of the peaks observed in the INS spectrum, besides the transverse and longitudinal magnetic susceptibility in the paramagnetic region.

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Abstract ID # 97
Magnetism &
Condensed Matter

Luís Gil

Observing the synthesis of a polymer brush, molecule by molecule

Densely surface-grafted polymers have attracted considerable attention due to the desirable interfacial properties that stem from both their conformation and anchored liquid-like state. To create these surfaces with desirable thicknesses and grafting densities a grafting-from approach, wherein polymers are grown from surface-attached initiators, must be used to assemble the layer. The most widely used polymerisation method for grafting-from approaches is Atom Transfer Radical Polymerisation (ATRP), due to its simplicity and versatility. The structure of such a layer is understood to modulate interactions between the coated surface and its local environment, including changes to lubrication, adhesion or fouling by contaminants. As such, understanding the structure of these polymer layers (including the molecular weight distribution of the substituent chains) is essential.

Prior neutron reflectometry (NR) work indicates the presence of a dense layer adjacent to the substrate, at the base of the brush. Gel permeation chromatography (GPC) studies and simulations of the ATRP process indicate that this layer consists of stunted polymer chains proximal to the surface. The alternative explanation that has been proposed is that this dense layer is made up of initiator moieties.

Here we observe the growth of a surface-initiated polymerisation in situ with NR; to our knowledge, this is the first time such an experiment has been performed. We show that the interior layer previously observed by NR is not due to a thick initiator layer, but rather a dense polymer layer that is formed during the initial stages of the polymerisation. This experiment paves the way for further kinetic experiments on PLATYPUS that seek to study the dynamic assembly of interfaces over timescales of 10 minutes to multiple hours.

*Abstract ID # 58
Chemistry &
Crystallography*

Isaac Gresham

Imaging the invisible: resolving polymer brush structure through a freeform Bayesian analysis of neutron reflectometry data

Surfaces covered with densely tethered polymer chains possess desirable properties and are ubiquitous in natural and human-made systems. These properties stem from the diffuse structure of these polymer brush interfaces; consequently, resolving their structure is key to better understanding and designing polymer brush systems. We have been using the PLATYPUS neutron reflectometer at the ACNS to achieve this structural resolution over the past six years, contributing to our understanding of brush structure, as well as fundamental polymer physics.

However, the analysis of collected reflectometry data is not without significant challenges; Inflexible models preclude viable structures and the uncertainty around accepted profiles (known as spread) is challenging to quantify. Furthermore, there is no guarantee of profile uniqueness in reflectivity analysis- multiple structures may match the data equally well. Quantifying profile uniqueness and determining the structures that agree with collected data (known as multimodality) has not been previously attempted on brush systems. Historically, data analyses have used least-squares approaches, which do not satisfactorily determine profile spread and bypass the possibility of multimodality.

Here we will briefly document our journey in modelling neutron reflectometry data collected from polymer brush systems, culminating in the presentation of our developed methodology. In this methodology, we model our brush with a freeform profile that minimises assumptions regarding polymer conformation while only producing physically reasonable structures. This model is built within *refnx*'s Bayesian statistical framework, which enables the characterisation of structural uncertainty and multimodality through Markov Chain Monte Carlo sampling. We demonstrate the rigour of our approach via a round-trip analysis of a simulated system before applying it to real data, examining the well-characterised collapse of a thermoresponsive brush. The method we describe is directly applicable to reflectometry experiments on soft and diffuse systems, but may also be generalised to other instruments where the "inverse problem" hampers data analysis.

*Abstract ID # 56
Neutron Instruments &
Techniques*

Isaac Gresham

Developments on the Platypus Neutron Reflectometer

PLATYPUS is the initial neutron reflectometer at the Australian Centre for Neutron Scattering with the capability to study surface and interface systems ranging from biomolecules, soft matter through to magnetic thin films [1-3]. There have been a number of significant improvements to both the instrument and data reduction and treatment software [4] over the last two years. On the hardware front the original detector has been replaced yielding higher count-rate capabilities, greater detection efficiency at shorter wavelengths and significantly lower background. The slits which define the neutron beam have been replaced with upgraded positioning mechanisms enabling greater flexibility in experimental setup. These changes have significantly enhanced the instrument performance with improved reproducibility. This presentation will highlight the enhancements and recent publications.

*Abstract ID # 43
Neutron Instruments &
Techniques*

Stephen Holt

Element Effects on High-Entropy Alloy Vacancy and Heterogeneous Lattice Distortion Subjected to Quasi-equilibrium Heating

We applied neutron diffraction and positron measurements to estimate the vacancy of CoCrFeNi and CoCrFeMnNi high-entropy alloys (HEAs) using Cu as a benchmark. The corresponding formation enthalpies and associated entropies of the HEAs and Cu were calculated. The vacancy-dependent effective free volumes in both CoCrFeNi and CoCrFeMnNi alloys are greater than those in Cu, implying the easier formation of vacancies by lattice structure relaxation of HEAs at elevated temperatures. Spatially resolved synchrotron X-ray measurements revealed different characteristics of CoCrFeNi and CoCrFeMnNi HEAs subjected to quasi-equilibrium conditions at high temperatures. Element-dependent behavior revealed by X-ray fluorescence (XRF) mapping indicates the effect of Mn on the Cantor Alloy.

*Abstract ID # 70
Advanced Materials*

E-Wen Huang

Progress with Hot Commissioning and First User Experiments on the SPATZ Neutron Reflectometer

The SPATZ neutron reflectometer was originally the V18 BioRef reflectometer at the BER-II Research Reactor (Berlin, Germany) [1, 2], and was transferred from HZB to ANSTO ownership during October 2016 to February 2017. The reflectometer was re-installed at ANSTO's 20 MW OPAL Research Reactor in the Neutron Guide Hall on the end position of the newly installed CG2B cold-neutron guide. The hot commissioning licence was issued in October 2018 with first neutrons in November 2018. Radiation surveys and shielding improvements were completed in May 2019. Since this time, hot commissioning has continued and has involved evaluating the performance of the instrument. SPATZ is a time-of-flight instrument, and the ability to translate chopper 2 makes the instrument highly configurable with the ability to select a time resolution from 1 to 12 %. A number of different sample environments have been tested including: solid-liquid cells with a HPLC pump for solvent contrast exchange, circulating water baths for temperature control, and the infrared spectrometer for simultaneous neutron reflectometry and ATR-FT-IR spectroscopy. The operating license was issued in December 2019, and first experiments are scheduled for the last quarter of 2020. SPATZ is now available for user proposals in the ACNS portal [3]. This presentation will highlight the instrument performance and achievements during hot commissioning and give an overview of the user program to date and first data collected.

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[2] M. Trapp et al., Rev. Sci. Instrum. **87**, 105112 (2016)

[3] <https://neutron.ansto.gov.au/>

*Abstract ID # 51
Neutron Instruments &
Techniques*

Tzu-Yen (Ian) Huang

New cell for studying porosity under mechanical and chemical stress

Tracking Changes in porosity at realistic underground conditions is of great scientific and technological interest to the resource industry, underground aquifer management, and material science, to name a few. Small Angle Neutron Scattering (SANS) and Ultra-Small Angle Neutron Scattering (USANS) are complementary techniques that can non-destructively investigate open and closed pore structure information in 2nm to 20 μ m range. The recent high-pressure cell developed by Blach is capable of applying uniaxial stress and fluid penetration of the sample with a pressure of up to 100MPa independently. This allows contrast matching and pore-fluid penetration to be studied at different mechanical loads. We report on our latest results from Quokka and Kookaburra, showing the effect of uniaxial strain on the porosity of tight shale rock. As we are in the process of extending the capability of the cell to temperatures above 500°C and adding triple axial strain capability, we also report on the optimization of sample thickness and windows. Moreover, we report on additional cell extension work that allows diffraction and X-ray/neutron Tomography to be used to study the samples. We are developing the new capabilities in cooperation with ANSTO, and we hope to have the system available to general users in 2022.

*Abstract ID # 101
Neutron Instruments &
Techniques*

Yeping Ji

Influence of tempering and surface grinding on the residual stress of 415SS laser clad hypereutectoid rail components

A growing reliance on critical transport infrastructure combined with the dependence upon railway for mining and mineral export has heightened operational requirements and lead to premature failure of rail components under severe loading conditions caused by plastic deformation, rolling contact fatigue and accelerated wear rates. Rail replacement is a costly and disruptive undertaking therefore in-situ maintenance is necessary for ongoing repairs to keep these extensive railway networks operational. Traditional maintenance techniques such as arc welding can be damaging to the rail and promote undesirable microstructural changes and softening due to the large thermal input. Laser cladding is an emerging regenerative maintenance strategy that utilises a high energy laser to metallurgically bond a deposition layer that imparts superior mechanical and tribological properties to restore the rail profile. Despite the smaller heat affected zone (HAZ) generated from the reduced thermal input, laser cladding produces a complex residual stress state due to thermal gradients, phase changes and solidification shrinkage. It is the combination of residual stress and cyclic wheel-rail contact stresses that govern the rail fatigue behaviour and susceptibility to wear and defect formation, therefore high internal stresses may increase the likelihood of failure.

415SS is a new martensitic stainless steel alloy developed to recondition hypereutectoid rail substrates and contains beneficial compressive stresses in the untempered cladding deposition, determined using neutron diffraction techniques. For in field applications, laser cladding repairs require further tempering and rail grinding procedures to prepare the surface for wheel contact by achieving the required mechanical properties and reducing surface roughness to minimise friction, wear and noise. Both thermal and machining processes alter the post cladding internal stress state which in turn impacts the fatigue behaviour.

Non-destructive neutron diffraction has been undertaken on the Kowari strain scanner at ANSTO to assess the effect of post cladding tempering and surface grinding on the residual stress of 415SS clad high carbon rail. The triaxial residual stress distribution was measured after 350oC and 540oC tempering processes and surface grinding to remove 0.5 mm and 1.4 mm from the cladding surface. Strain scanning was also performed on a disc with a 0.4µm surface finish. The research outcomes from this investigation will assist in better understanding the effect of post cladding processes on the rail fatigue behaviour as accurate measurement of the internal stress state is a critical aspect in developing a viable laser cladding maintenance strategy. These findings will be used in conjunction with full microstructural and mechanical property evaluation to determine the influence of cladding repairs on rail performance and identify the most desirable parameters for post cladding procedures to optimise the operation lifetime of rail components.

*Abstract ID # 73
Manufacturing &
Engineering*

Olivia Kendall

TBAB semi-clathrates studied by Quasi Elastic Neutron Scattering (QENS) using Emu, the high resolution backscattering spectrometer at ANSTO

Potential applications for gas hydrates include gas purification, water desalination, and CO₂ capture that is possibly combined with methane extraction. All of these rely on the high selectivity of the guest gas molecules in hydrates. It has been shown, that the addition of TBAB (i.e. Tetra-n-butyl ammonium bromide) softens the thermodynamic conditions of gas hydrate formation without compromising the CO₂ selectivity, a substantial benefit in reducing the carbon output from existing fossil-fuel power plants.

The hydrate structure formed using TBAB is known as a semi-clathrate which differs from the more common clathrate structures that are formed from pure water and gas. For common clathrate structures (sI, sII, or sH) only the gas molecules are entrapped in the cavities of the water structure. Semi-clathrates generally crystallize into two structure types known as type A and B. The Br-anion of TBAB participates to the water molecule framework, while the tetra n-butyl cation is located at the center of 4 large cages. Additional smaller cavities are available for the enclathration of gas molecules. It has been shown recently that these cavities are distorted by the inclusion of guest molecules like CO₂ (Muromachi et al., 2014).

We present here our first quasi-elastic neutron scattering (QENS) results for TBAB semi-clathrates formed with type A and B using the EMU backscattering spectrometer at ANSTO. This technique is well suited to studying the libration of the butyl chains confined within the host cages, and how the slow dynamics changes with the enclathration of CO₂ molecules. Neutron diffraction was applied on the same samples in order to confirm their crystallographic structure.

QENS measurements are highly sensitive to hydrogen (H) atoms while being very insensitive to the deuterated (D) atoms. As well, the method is also insensitive to the dynamics of CO₂ molecules. We use these characteristics to suppress scattering from the water framework by making it from D₂O rather than H₂O. As a result, only the dynamics of the n-butyl chains are observed. Early results suggest the interaction of the CO₂ molecules with the mobile butyl chains is key to the improved selectivity of TBAB semi-clathrates.

References:

S. Muromachi, K.A. Udachin, K. Shin, S. Alavi, I.L. Moudrakovski, R. Ohmura, J.A. Ripmeester, Guest-induced symmetry lowering of an ionic clathrate material for carbon capture, Chem. Commun. 50 (2014) 11476–11479

Abstract ID # 74
Chemistry &
Crystallography

Alice Klapproth

Poly(vinyl alcohol) and Functionalized Ionic Liquid-Based Smart Hydrogels for Doxorubicin Release

Limitations associated with the traditional cancer therapies prompt the scientific community to develop effective, safer, smarter, and targeted drug carriers that improve the efficiency of the drug carrier, reduce the adverse effects of the drug on the healthy cells, and help in preventing the cancer recurrences. This research aims to design a stimuli-responsive, self-healable, adhesive, and injectable polymeric hydrogel with an ester-functionalized ionic liquid as one of the additives to improve the efficiency of the anticancer drug in encapsulation and localized delivery. The designed polymeric hydrogel responds to intracellular biological stimuli (e.g., acidic pH of cancerous cells and temperature), changes the morphology through changing the shape and size of the gelator within the hydrogel matrix, and releases encapsulated doxorubicin (DOX) at the tumor site efficiently. Molecular interactions, gel morphology, and mechanical strength of the hydrogel were characterized through various analytical techniques, including small-angle neutron scattering. Adhesive properties of the polymeric hydrogel were measured by lap-shear strength tests and the biocompatibility and cellular drug uptake study on human breast cancer (MCF-7) and human cervical carcinoma cells (HeLa). The in vitro cytotoxicity and drug release study showed that the hybrid hydrogel is more effective at killing the cancerous cells, and the targeted release of DOX occurred at intracellular acidic pH. The polymeric hydrogel provides an efficient therapeutic approach for the encapsulation and release of the drug. Overall, the study offers a proof of concept to test the feasibility of the hydrogel system whether the hydrogel formulation helped or hindered the total cellular DOX trafficking.

Abstract ID # 24
Advanced Materials

Muzammil Kuddushi

Scientific computing support for neutron scattering experiments at ANSTO

The purpose of the scientific computing support at ANSTO is to aid in the interpretation of both structural and dynamical data from the neutron scattering instruments using atomistic modelling calculations. Most of these calculations are done with ab initio scientific software packages based on Density Functional Theory, including VASP, WIEN2K, ABINIT, SIESTA, PHONON, and QUANTUM ESPRESSO, although some are performed with packages based on classical force fields, such as LAMMPS, DL_POLY, NAMD, and GULP. Analysis of the results of these calculations exploits tools such as VMD, NMOLDYN, XCRYSDEN, and ISAACS, in addition to in-house code.

Calculations and analysis are carried out locally on a scientific computing Linux cluster comprising both ACNS dedicated cores and ANSTO shared ones, with jobs managed by PBS. We give a brief overview of all of the above capabilities and an example of a typical calculation/analysis.

*Abstract ID # 45
Neutron Instruments &
Techniques*

Ramzi Kutteh

Topological barrier for skyrmion lattice formation in MnSi

We report the observation of a topological skyrmion energy barrier through a hysteresis of the skyrmion lattice in the prototypical helimagnet MnSi. Measurements of the energy barrier were made using small-angle neutron scattering and a bespoke DC field coil to allow for high-precision hysteresis loops. Data has been analyzed using an adapted Preisach model to quantify the energy barrier for skyrmion formation and the magnetic behavior of the sample as a whole. This analysis was then compared with minimum-energy path analysis based on atomistic spin simulations to verify the topological nature of the barrier. This reveals that the skyrmion lattice in MnSi forms with an activation barrier of several eV and in domains that are several hundred skyrmions in size.

*Abstract ID # 8
Magnetism &
Condensed Matter*

Allan Leishman

Synthesis and structure of ALaTiO_4 and $\text{A}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ ($\text{A} = \text{Na}^{+}, \text{K}^{+}$) Ruddlesden-Popper type photocatalysts

Global warming is a current hot topic due to its potential for irreversible environmental damage. Ambitions were made within the Paris agreement to limit the temperature rise to be below 1.5°C pre-industrial level. Alternative fuel sources are needed to replace fossil fuel, reducing the emission of greenhouse gases including CO_2 . Hydrogen gas is one popular choice to replace fossil fuels, due to its high energy density per unit weight, with existing technologies utilising hydrogen as energy generator. Hydrogen can be generated renewably by sunlight driven, photocatalytic water-splitting. Metal oxides, including those with a Ruddlesden-Popper type structures are being studied as potential photocatalysts. The structure's multiple cationic sites, which allows for different combinations of metal cations that can be used to adjust the bandgap. The layered structuring also allows for the intercalation of different cations within the structure that allows for modifications post synthesis. KLaTiO_4 is a $n=1$ Ruddlesden-Popper type layered perovskite. KLaTiO_4 can be used as a Hydrogen Evolution Catalyst (HEC), producing $9.540 \text{ } \mu\text{mol}$ of H_2 gas per hour from 20 mg of catalyst, when using methanol as sacrificial electron donor and platinum co-catalyst.

KLaTiO_4 was prepared using traditional solid-state chemistry methods to provide a sample for both catalytic testing and structural studies using neutron diffraction. Synthesis of KLaTiO_4 above 900°C resulted in the presence of $\text{K}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ impurity in the product. $\text{K}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ is structurally similar to KLaTiO_4 , both being layered perovskite of the Ruddlesden-Popper type structure, with layers of TiO_6 . The main difference between the two is KLaTiO_4 has 1-layer of perovskite-like TiO_6 blocks, while $\text{K}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ has 3-layer perovskite slabs. The sodium analogues, NaLaTiO_4 and $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ can also be made and these are isostructural to their potassium counterparts. In this presentation, two factors important for the synthesis of ALaTiO_4 and $\text{A}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ ($\text{A} = \text{Na}^{+}, \text{K}^{+}$) will be discussed. The first factor to consider is the volatility of alkaline metal ions at elevated temperatures. Due to this volatility, excess Na or K needs to be included in the initial reagent mixture. Ex-situ XRD measurements showed that if the excess of Na_2CO_3 was limited to 10%, neither NaLaTiO_4 nor $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ could be made. Successful synthesis of NaLaTiO_4 or $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ required 50 % (minimum tested) alkaline metal reagent excess. The second factor to consider is related to sintering temperature. Multiple samples of NaLaTiO_4 or $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ were made using traditional solid-state synthesis methods at temperature between 750°C to 950°C . Incomplete reaction was observed if the temperature was kept below 750°C during the synthesis, XRD revealing unreacted La_2O_3 , as well as other unidentified impurities. It was also discovered that when reagents with the stoichiometry to make NaLaTiO_4 (with Na_2CO_3 excess) were sintered above 900°C $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ impurities were present, which is a lower temperature than most literature reports. Finally, $\text{Na}_2\text{La}_2\text{Ti}_3\text{O}_{10}$ was made at 800°C , which is lower than other literature reports, and the temperature which NaLaTiO_4 was found to be made at good purity.

Abstract ID # 9
Chemistry &
Crystallography

Junwei Li

A high-performance and long-cycle-life spinel lithium-ion battery cathode achieved by site-selective doping

Lithium-ion batteries (LIBs) form an important part of our daily life, powering portable electronic devices, as well as electric and hybrid electric vehicles. However, the limited energy density of current LIBs results in their failure to meet the increasing requirements of rapidly developing technologies. Since the performance limitation in existing LIB technology is the cathode, exploring high-energy-density cathode candidates becomes extremely important. Spinel $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO) is considered one of the most promising cathode materials for next-generation high energy-density LIBs, owing to its high operating voltage of 4.7 V vs. Li, low fabrication cost, and high energy density approaching 650 Wh kg⁻¹, which is beyond that of most other LIB cathode materials, such as LiFePO_4 at ~560 Wh kg⁻¹, LiMn_2O_4 at ~480 Wh kg⁻¹, and $\text{LiMn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1/3}\text{O}_2$ at ~510 Wh kg⁻¹. Unfortunately, LNMO suffers from rapid capacity decay and unsatisfactory cycle stability, limiting its practical application and commercialization. Various doping strategies have been widely adopted to enhance the electrochemical stability of LNMO. Although the electrochemical performance of LNMO is enhanced through doping, the mechanism by which the performance is improved remains unclear, with the chemistry- and structure-function relationships for chemically modified LNMOs relatively unknown. In this work, we not only demonstrate a site-selective doping strategy for an easily-prepared high-performance LNMO cathode through Mg doping, but also comprehensively reveal the underlying enhancement mechanisms using a series of in operando and ex situ characterization techniques. Mg dopants, selectively residing at 8a and 16c sites of the Fd-3m structure, change the way how LNMO responds to the lithium intercalation and de-intercalation during charge-discharge processes. Meanwhile, the addition of Mg ions at such sites significantly prohibits the partially-irreversible two-phase behavior of LNMO, mitigates against the dissolution of transition metals, thus preventing the formation of the undesirable rock-salt phase and reducing the Jahn-Teller distortion and voltage polarization, consequently offering the extraordinary structure stability to LNMO. Consequently, the modified LNMO exhibits excellent extended-long-term electrochemical performance, retaining ~86 % and ~87 % of initial capacity after 1500 cycles at 1 C and 2200 cycles at 10 C, respectively in half cell configuration, which is reported for the first time and demonstrates their great commercial potential. Such excellent cycle and rate performance are also reflected in a prototype full-battery with a novel TiNb_2O_7 counter electrode. This work provides a new strategy for the chemical modification of electrode materials that may be applied more generally in battery researches, whereby dopants may be used strategically to address specific electrode issues.

Abstract ID # 94
Advanced Materials

Gemeng Liang

Lead-free (Ag,K)NbO₃ materials for high-performance energy conversion

Explosive energy conversion materials with extremely rapid response times have a diverse and growing range of applications in energy, medical, and mining areas. Research into the underlying mechanisms and the search for new candidate materials is so limited that Pb_{0.99}(Zr_{0.95}Ti_{0.05})_{0.98}Nb_{0.02}O₃ is still the dominant material after half a century. In this work, we report the discovery of a new, lead-free ferroelectric material, (Ag_{0.935}K_{0.065})NbO₃ for explosive energy conversion applications. This material not only possesses a record-high energy storage density of 5.401 J/g, but also exhibits excellent temperature stability (up to a disruptive ferroelectric to ferroelectric phase transition at 150°C) by comparison with Pb_{0.99}(Zr_{0.95}Ti_{0.05})_{0.98}Nb_{0.02}O₃ (which exhibits the ferroelectric to ferroelectric phase transition but at the much lower temperature of 41~70°C). (Ag_{0.935}K_{0.065})NbO₃ enables extremely high power, energy conversion within 1.8 microseconds, generating a pulse with e.g. a current ~ 22 A. Furthermore, pressure-dependent physical characterization, together with transmission electron microscopy, in-situ neutron diffraction analysis and theoretical modelling, reveals the mechanism underlying the observed explosive energy conversion behavior. It is found that the fast release of the stored energy can be attributed to a pressure-induced octahedral tilt change from a-a-c+ to AgNbO₃-type a-a-c-/a-a-c+, in accordance with an irreversible pressure driven FE-AFE phase transition. This work provides not only an alternative (with significantly better performance) to the current commercially-employed lead-containing materials, but also provides guidance for the further development of new materials and devices for explosive energy conversion applications.

Abstract ID # 12
Advanced Materials

Zhen Liu

In situ Neutron Diffraction Study on Layered Oxides $\text{Na}_{0.5}\text{Ni}_{0.25}\text{Mn}_{0.75}\text{O}_2$

Layered oxides based on first-row transition metals dominate cathode materials for commercial batteries and remain highly interesting as well as challenging in their structural study during electrochemical reactions. Neutron diffraction is a powerful method to obtain periodic structural information complementary to that obtained by X-ray diffraction. Although inferior to X-ray diffraction in signal resolution, neutron diffraction reveals more reliable structural evolution as the whole bulk of materials are fluxed with neutron beam. $\text{Na}_{0.5}\text{Ni}_{0.25}\text{Mn}_{0.75}\text{O}_2$ is a potential sodium ion battery cathode due to its high operating voltage 3.2 V vs Na^+/Na and high capacity 130 mAh/g. Its stoichiometry is designed to only utilize the redox couple $\text{Ni}^{4+}/\text{Ni}^{2+}$ to avoid the unstable redox couple $\text{Mn}^{4+}/\text{Mn}^{3+}$. The high voltage phase for this material has been under debate. The fact that sodium-containing layered oxides are highly hydroscopic, especially at low sodium content, makes it hard to study the final phase ex situ. In the work presented here, we have pushed the signal resolution of in situ neutron diffraction to the limit by loading the optimized material mass at the positive side and the corresponding amount of amorphous hard carbon at the negative side of a pouch cell. The result is the first robust proof of the reversible structural evolution from P3, O3 to O3s on charging and back to O3, P3 on discharging.

*Abstract ID # 14
Advanced Materials*

Jiatu Liu

Multilayers of doped Silicon are the heart of the diodes and transistors which form the basis for virtually all modern electronics. With a rapidly impending need for more energy efficient computers, it is interesting to see what can be done with multilayers of more exotic starting materials. The superconductor sandwiches we study are thin-film multi-layers of the high temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$ and the perovskite manganite $\text{Nd}_{0.65}(\text{Ca}_{0.7}\text{Sr}_{0.3})_{0.35}\text{MnO}_3$. We discovered that a highly unusual superconducting state could be induced in the $\text{YBa}_2\text{Cu}_3\text{O}_7$ by tuning the properties of the manganite. It remains to be determined precisely how the manganite can so radically effect the superconducting state in the adjacent layer. Here, we discuss our current polarised neutron reflectivity (PLATAPUS) and Bragg scattering (TAIPAN) work to investigate the role of the manganite's magnetism and magnetic ordering in causing the unusual properties of the superconductor sandwiches.

*Abstract ID # 19Neutron
Magnetism &
Condensed Matter*

Ben Mallett

The Australian Centre for Neutron Scattering offers neutron spin filters for six instruments (WOMBAT, PELICAN, QUOKKA, PLATYPUS, TAIPAN and SIKA), using a combination of supermirrors and polarised ^3He cells. The infrastructure required to use ^3He spin filters is particularly complicated, and a clear understanding of this is pivotal to designing and carrying out successful experiments which take advantage of polarised neutron scattering. Such experiments typically investigate systems where detailed study of magnetic effects or the separation of coherent and incoherent scattering is needed.

Here, the capabilities for polarised neutron scattering experiments for each of these instruments are summarised, including compatible sample environments such as cryostats, magnets and sample changers, and a discussion of key considerations when planning experiments using polarised neutrons. A newly-acquired 7 tesla compensated vertical magnet will also be described, and some initial results for its use on the SANS instrument QUOKKA will be presented. Finally, some possible future directions to further develop the polarised neutron capabilities at ACNS are outlined.

*Abstract ID # 25
Neutron Instruments &
Techniques*

Andrew Manning

Understanding disorder in the $\text{Y}_2\text{Sn}_2\text{-xZrxO}_7$ pyrochlore oxides

Solid oxide fuel cells (SOFCs) offer clean alternatives to current carbon emitting energy sources; however, reducing their operation temperature is a major challenge for widespread application. Hence, the development of novel electrolyte materials with high room temperature ionic conductivity is crucial. Pyrochlore oxides, of the general chemical formula $\text{A}_2\text{B}_2\text{O}_7$, exhibit chemical and structural flexibility, resulting in a diverse range of physical properties and technological applications, such as host matrices in the immobilization of actinide-rich nuclear wastes. In particular, they have gained interest as fast-ion conductors for electrolytes in SOFCs.

The pyrochlore structure is highly ordered, which limits long-range oxygen diffusion. This can be altered via disordering, which results in the formation of oxygen Frenkel pairs that improve conductivity. The pyrochlore structure can adopt the disordered-fluorite structure via changes in composition, temperature, pressure and radiation. The disordered-fluorite exhibits lower formation energy of the Frenkel defect; however, this increase in structural disorder can increase the activation energies needed for long-range migration, which results in optimal conductivity occurring in partially disordered materials. Hence, the interplay between disorder and order in the atomic structure is key to the physical properties of these materials.

There have been many studies dedicated to understanding the structural order and disorder in pyrochlore and disordered-fluorite oxides, with a recent study claiming the local structure of the disordered-fluorite to be weberite. It was proposed that the overall structure of a disordered-fluorite consists of randomly arranged orthorhombic weberite domains that result in the long-range cubic disordered-fluorite.

In this study we use low temperature (15 K) neutron pair distribution function (PDF) and big box modelling to understand the local-scale structure of the $\text{Y}_2\text{Sn}_2\text{-xZrxO}_7$ system. We show that the local structure of the $\text{Y}_2\text{Zr}_2\text{O}_7$ disordered fluorite does not contain ordered weberite domains, which emphasizes the importance of low temperature measurements in the local structure analysis of disordered oxide materials. Our analysis of the $\text{Y}_2\text{Sn}_2\text{-xZrxO}_7$ series serves as a direct method for quantifying disorder and Frenkel defects. Understanding and quantifying these atomic-scale distortions is essential in simulations and design as it directly influences the energy landscape for anion mobility. These techniques can be used in the development and engineering of novel and advanced electrolyte materials for SOFCs.

*Abstract ID # 15
Advanced Materials*

Frederick Marlton

Neutron Laue Diffraction - A spotted history, a scintillating future

In 1912, Max von Laue first demonstrated atomic diffraction reduced by passing a beam of polychromatic X-rays through a single crystal [1], and was awarded the Nobel Prize for Physics two years later for his discovery. Laue diffraction, as this phenomenon was later called, was also demonstrated with neutrons [2], shortly after the pioneering monochromatic experiments by Schull and co-workers at Oak Ridge in the 1940s. The Laue technique largely languished for many decades however, due to the perception that harmonic overlap and complicated wavelength-dependent corrections yielded data of lesser quality than monochromatic diffraction.

The extreme demands of protein crystallography for higher data collection rates, for both X-rays [3,4] and neutrons [5], coupled with high-resolution, large area detectors, and powerful image-analysis techniques, allowed Laue diffraction on a continuous source of radiation to return to the forefront of crystallography in terms of increasing unit-cell size, decreasing sample volume, and higher-throughput experiments, advantages that translate directly to chemical crystallography, materials science, and exotic physics [6]. Modern reactor-based neutron Laue diffractometers with large image-plate detectors permit extensive continuous sampling of reciprocal space with high resolution in the two-dimensional projection and a wide dynamic range with negligible bleeding of intense diffraction spots, qualities that are highly suited to detection of incommensurate structures, high-pressure crystallography, and diffuse scattering.

Although time-of-flight (TOF) neutron diffraction on a white beam was first demonstrated at the Dubna pulsed reactor in 1964 [7], it was not until a position-sensitive (scintillation) detector became available that the full utility of the technique for single-crystals could be realised in a landmark experiment at IPNS in 1984 [8]. Using a scintillator gave negligible parallax, which allowed the detector to be moved close to the sample to increase significantly the solid angle of detection and thereby make the data-collection efficiency comparable to that on a monochromatic diffractometer with a point detector at a reactor source. Such detector developments [9] will continue to play a key role in broadening the application of neutron Laue diffraction.

A survey of pioneering studies of neutron Laue diffraction in the recent past at reactors and spallation sources guides us to what we can expect to achieve with upcoming instrumental and data-analysis advances.

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Abstract ID # 109
Neutron Instruments &
Techniques

Garry McIntyre

Magnetic properties of the porous coordination polymer $\text{Ni}_3(\text{OH})_2(\text{C}_4\text{O}_4)_2 \cdot 3\text{D}_2\text{O}$

The magnetism of porous coordination polymers is of long standing interest as changes to the hydration level of the pore have been shown to drive small changes in the structure of the framework, which in turn give rise to large differences in the magnetic properties. This capacity for magneto-structural correlations naturally leads to ideas such as utilising these properties as a magnetic switch or sensor, but also allude to the ability of tuning the magnetic properties of the material. In the current contribution, I will report on the characterisation of $\text{Ni}_3(\text{OH})_2(\text{C}_4\text{O}_4)_2 \cdot 3\text{D}_2\text{O}$. This porous coordination polymer has a magnetic topology where chains of alternating edge and vertex coupled triangles display ferromagnetic exchange interactions. These chains are then coupled antiferromagnetically. Application of small magnetic fields can give rise to a ferromagnetic state, but unusually this does not display a magnetic hysteresis. The magnetic phase diagram also shows some other unconventional behaviour. We have performed inelastic neutron scattering experiments on this materials using the Pelican time-of-flight spectrometer and have analysed the data using linear spin wave theory.

*Abstract ID # 64
Magnetism &
Condensed Matter*

Richard Mole

Disorder By Design: Long- and Short-Range Pyrochlore Ordering

Carbon-neutral energy generation is being developed in order to combat climate change. Two technologies of current interest, which are related to renewable and nuclear energy respectively, are next-generation oxygen-ion conductors for fuel cells and materials suitable for long-term storage and disposal of radioactive nuclear wastes [1-2].

Pyrochlores of the structure $A_2B_2O_7$ have found immense applications in each of the above areas. Ionic conductors for fuel cells require flexibility and movement in their anionic sublattice, whereas the storage of radioactive nuclear wastes needs a robust lattice from which ions cannot escape. This is a seemingly contradiction in requirements. It is believed that the oxygen vacancies present in the pyrochlore structure allow for the development of short-range disorder, whilst keeping the long-range order intact [3].

The pyrochlore structure can be viewed as a superstructure of the defect-fluorite structure. The defect-fluorite structure (A_2BO_5) consists of a random distribution of cations and oxygen vacancies. However, by choosing A and B with a particular ionic radii ratio, the ordered pyrochlore superstructure may form under ambient conditions. This ordering of oxygen vacancies may be analysed using neutron powder diffraction and used to reason the enhanced properties and applications of pyrochlores [4].

The current work aims to characterise oxygen-vacancy disorder in defect pyrochlores so to enable the rational design of defect pyrochlores that are optimised for specific applications. We have done this by looking at 'stuffed' pyrochlores of the form $A_2(B_2-xAx)O_{7-x/2}$ where the smaller B-type cation, in this case Ti^{4+} , is progressively replaced by a larger A-type cation (Tm^{3+}). We wish to determine whether controlling the disorder in the cation sublattice will allow us to tailor-make stuffed pyrochlores targeting specific applications across ionic conductivity, magnetism, photocatalysis and the storage of long-term radioactive waste.

Series of stuffed pyrochlores have been synthesised using conventional solid-state methods and their long-range average structures characterised by Rietveld refinement against combined neutron and synchrotron X-ray diffraction data. The local short-range order has been characterised by Raman spectroscopy and XANES. Other measurements have also been performed regarding their applications, demonstrating a vast improvement in their ionic conductivity at high temperatures.

These results will be presented, along with a judgement as to whether inducing certain types of disorder within the pyrochlore structure can lead to them being purposely engineered for specific applications.

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*Abstract ID # 54
Chemistry &
Crystallography*

Bryce Mullens

Hydrogels with tuneable dissipation for mechanotransduction studies

There is a need for the development of hydrogel substrates with tuneable dissipation properties for various applications such as orthopedic load-bearing applications and scaffolds for cell culture. Tuning of stiffness and toughness by using double network gels consisting of two polymer networks has been explored for such applications. However, the mechanical properties of such hydrogels are often hindered by swelling. Moreover, the development of hydrogels with stable mechanical properties and tuning of dissipation in such hydrogels remains a challenge. Recently, there has been considerable research interest in using hydrogels with tuneable loss modulus, or dissipation properties as substrates in studies of cellular mechanotransduction.

In our research, we explored the influence of polymerizing monomers inside a crosslinked polymer network. The second networks were designed to hydrogen bond with the first crosslinked polymer network. Specifically, we used acrylic acid and tannic acid as monomers which are polymerized inside a crosslinked gel to form linear poly(acrylic acid) chains and oligomeric poly(tannic acid), respectively. We systematically studied the mechanical properties of these two gels using tensile and compression tests. The hydrogels exhibited high stiffness and toughness, and the results can be attributed to the density of the hydrogen bonds between the polymers in the gel. As a proof of concept, we tested the possibility of producing gels with tuneable loss modulus without significant variations in the storage modulus by polymerizing the monomers under a printed UV mask. The obtained mechanical properties were studied using rheology. Finally, we tested the stability of such gels in cell culture conditions (37 °C, PBS). We envisage that such hydrogel substrates will be helpful in studying cells' responses to different levels of loss modulus and loss modulus gradients. In future work, we plan to attach adhesion ligands on such substrates and investigate the combined effect of mechanical properties and ligand density on mechanotransduction.

*Abstract ID # 27
Advanced Materials*

**Badri
Narayanan Narasimhan**

refnx - The Next Generation of Reflectometry Analysis Software

refnx [1] is a next generation reflectometry analysis package, building on its predecessor, Motofit. In this presentation we discuss its main design features:

- Bayesian statistics core with comprehensive uncertainty analyses and model selection ("how many layers can the data justify") [2].
- modular construction of structural models, ranging from a basic Slab up to freeform SLD profiles and Lipid membrane leaflets. These components are easily extensible.
- Co-refinement of multiple contrast datasets.
- Mixed Area models.
- Python based with analyses performed in Jupyter notebooks or a Qt GUI.

refnx is specifically designed to facilitate reproducible research. Here we also discuss what reproducible research means in the context of a neutron scattering study, outlining how this is achieved with refnx, and how these practices could (should) be taken up by neutron scatterers in general.

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refnx: neutron and X-ray reflectometry analysis in Python
Journal of Applied Crystallography, 2019, 52, 193-200

[2] If you don't know what Bayesian statistics is and have always wondered, you'll now find out.

*Abstract ID # 30
Neutron Instruments &
Techniques*

Andrew Nelson

Unconventional hydrocarbon resources have been of large interest in recent years, hence, there are greater needs for more accurate estimations of gas reserve in the reservoirs. Although researchers use the SANS technique to investigate open and closed porosity in rocks routinely, the effects of nanopore condensation is not well understood. This study investigates the behavior of deuterated methane (CD₄) in the nanopore at different gas pressures using SANS. Silica aerogel was chosen as the sample for this study due to the assumed similarity in its composition to sandstone which mainly consists of quartz. However, the aerogel is a synthetic material with a totally opened pore structure and the lack of impurities, which prevents other factors from affecting the interaction between CD₄ and the pores. We plan to use the aerogel result to work on a model of methane condensation in nanopores which then can be used to evaluate the extent of this phenomenon in real rocks. We also show how the application of contrast matching measurements revealed the pore structure of the aerogel we studied at larger scales where the features of the aerogel matrix were not as expected and were limited to certain sizes rather than exhibiting a fractal behavior found in previous SANS measurements of aerogels.

*Abstract ID # 96
Earth & Environment*

Phung Nhu Hao Vu

Giant shifts of crystal field excitations with temperature as a consequence of internal magnetic exchange interactions

Crystal field theory, invented in the 1930s by Hans Bethe, provides an explanation of the crystal field excitations (CFE) observed in inelastic neutron scattering (INS) spectra of rare-earth compounds [1]. However, some long withstanding problems remain. Our inelastic neutron scattering experiments on vanadates CeVO₃ and TbVO₃ did reveal an unexpected large shift of the energies of the crystal field excitations as a function of temperature. Thus far, only few publications on INS experiments mention shifts in crystal field excitation (CFE) energy in spectra above and below magnetic phase transition temperatures [2,3,4]. Recent IR transmission measurements also identified a CFE energy shift in hexagonal DyMnO₃ with temperature and upon the application of an external magnetic field [5]. However, no studies report a detailed microscopic theory and to the best of our knowledge does not exist in literature.

The vanadates CeVO₃ and TbVO₃ share the same orthorhombic Pbnm crystallographic structure featuring tilted, corner-sharing octahedra and possess a Cz-type antiferromagnetic structure below Néel temperatures 124 K and 110 K, respectively [6-9]. In both vanadates the CFE energies shift strongly below the magnetic phase transitions.

We have used quantum-mechanical point-charge calculations to determine the energies of observed CFEs to model their large shift as a function of temperature. Two mechanisms have been simulated: (i) distortions of the crystallographic lattice due to magnetostriction, or (ii) internal magnetic exchange interactions with CF levels at the onset of the magnetic order. The effect of lattice distortions measured by neutron diffraction [7,8] produces a negligibly small shift of CFE energy, therefore cannot drive the shift. Results accounting for internal magnetic exchange fields arising from the ordered V³⁺ spins reveal a shift which agrees excellently with neutron data. The CFE energy shift is well reproduced with the same shift in CFE energy and intensity. Therefore, the unexpected large shift of CFE energies with temperature has been confirmed by point-charge model theoretical calculations and can be attributed to an internal magnetic exchange interaction.

In addition to the CFEs, spin-wave excitations (magnons) are present in both vanadate materials below the magnetic phase transition. In TbVO₃ there appears to be an anticrossing-like behaviour between magnon and CFE at 14 meV. Such an anticrossing has been reported in far-IR transmission investigations in Tb₃Fe₅O₁₂ garnet [12]. In order to investigate this observation in TbVO₃, magnon dispersion calculations have been performed to clarify the exact nature of the interaction.

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Abstract ID # 108
Magnetism &
Condensed Matter

Joel O'Brien

Investigating methods of minting Ancient Greek silver plated copper coins: studies in Neutron Tomography, Texture and Phase Analysis.

Neutron tomographic, texture and phase analyses undertaken on the Neutron Beam Instruments Dingo, Kowari and Echidna have been employed to investigate plated silver coins minted in Athens and in the Greek colonies of Kroton and Metapontum (Southern Italy) during the 6th and 5th centuries BC. The investigation aims to define the plating method by characterising the manufacturing conditions and morphological and structural features of the specimens. Thickness maps of the silver plating and porosity give an indication on the similarity of the production techniques. The texture analysis gives an indication on the mechanical processes and temperature under which these coins were struck. The status of these coins is uncertain: were they official issues by state-authorities during periods of silver shortages or the product of ancient or modern counterfeiters?

Abstract ID # 38
Cultural Heritage

Scott Olsen

Insights into doped trirutiline structures gained through neutron diffraction

Metal oxides of formula MSb_2O_6 have garnered widespread interest in materials science research as they prove to be promising materials as semiconductor photocatalysts and ionic conductors. [1] Many of these compounds (e.g. $M = Co, Zn, Ni, Fe$ etc.) are known to crystallize in a tetragonal trirutile phase [2], although $CuSb_2O_6$ is known to exhibit a monoclinic distortion. [3] We are investigating several ternary compounds with general formula AB_2O_6 , with substitutional doping of A ($Cu_{1-x}Ni_xSb_2O_6$) and B ($ZnSb_{2-x}Sn_xO_6$).

Preliminary results have shown us that these materials show promising behavior as mixed ionic conductors due to oxygen vacancies being created through the substitutional doping. These were confirmed through neutron diffraction experiments conducted at the Australian Centre for Neutron Scattering. An unexpected mixed occupation of M/Sb positions was also revealed in these experiments.

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*Abstract ID # 31
Chemistry &
Crystallography*

Sneh Patel

Interactions at interfaces of magnetic materials such as giant magnetoresistance (GMR) form the physical foundation of many technological devices in today's market. Although GMR technologies are now somewhat dated, interactions at the interface between layers of oxide materials continue to demonstrate attractive mechanisms for technology applications due to the wide variety of available oxide materials as well as their ability to be well lattice-matched to form heterostructures.

Magnetic thin-film superlattices made of 15 repetitions of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ (LSMO) and LaNiO_3 (LNO) have been shown to exhibit a magnetic exchange interaction in LNO that is dependent upon its thickness n (where n is the number of unit cells of LNO) between LSMO layers [1]. At $n=1$, the LSMO layers are ferromagnetically aligned with each other. At $n=3$ however, the LSMO layers are canted by 110° with respect to one another. This canting is reportedly driven by an emergent c -axis spin-helix in LNO that arises due to charge transfer at the interfaces between LNO and LSMO [2].

We have fabricated superlattices of similar quality to Ref. [1] using Reflected High Energy Electron Diffraction (RHEED) assisted Pulsed Laser Deposition (PLD), where RHEED is used to ensure unit-cell precision in layer thicknesses. These superlattices have been designed so they exhibit $n=3$ and $n=1$ interactions within the same superlattice in a modulated pattern. This modulation of the effective LNO exchange interaction in these samples creates a toy model of coupled magnetic layers to explore. The modulated design of these samples create "frustrated" environments where the effective exchange interaction is different on each side of an LSMO layer within the superlattice. We utilise polarised neutron reflectometry using PLAYPUS to reveal the complex magnetic profile of these modulated superlattices by measuring the non-spin-flip (R_{++} , R_{--}), and spin-flip (R_{+-} , R_{-+}) cross sections. Presented are the current progress and prospects in the fitting process of these complex datasets.

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*Abstract ID # 78
Magnetism &
Condensed Matter*

Oliver Paull

Koala, a versatile single-crystal diffractometer

KOALA is a versatile diffractometer for neutron single-crystal diffraction studies on a wide range of applications in chemistry, materials science and physics. Of the many user experiments published from KOALA data, we present two case studies related to materials science and physics.

The $S=\frac{1}{2}$ helical-honeycomb antiferromagnet α -Cu₂V₂O₇ shows a broad peak in its magnetic susceptibility ~ 50 K followed by an abrupt increase below 33 K, indicative of a phase transition to a magnetically ordered state. Neutron diffraction reveals that $S=\frac{1}{2}$ Cu²⁺ spins are antiferromagnetically aligning with an ordered moment of 0.93(9) μ B, predominantly along the crystallographic a axis.

The photovoltaic materials MAPbX₃ (MA = CH₃NH₃; X = Cl, Br, I) are widely studied due to their high conversion efficiencies. NMR spectra indicates dynamic reorientation of the MA ion, suggesting tumbling within the perovskite cage with only the amine end of the group interacting with the inorganic network. Single-crystal neutron diffraction was used to refinement all three structures for comparison. In each case, the MA group is disordered and surrounded by halogen ions with anisotropic displacement ellipsoids. However, for the Br and Cl structures small anomalies were observed in the probability density of the lead ions, possibly indicating a ferroelectric-like behaviour or a subtle difference in symmetry.

*Abstract ID # 77
Neutron Instruments &
Techniques*

Ross O. Piltz

Understanding the structural disorder of (Ag_xCu_{1-x})₂ZnSnSe₄ based Kesterite semiconductor by neutron diffraction study.

The quaternary semiconductor Cu₂ZnSnSe₄ (CZTSe) is a promising environment-friendly and low-cost material as a solar cell absorber layer with a power conversion efficiency of 11.6%. Its photovoltaic performance is currently limited due to its disorder between the Copper & Zinc lattice sites, which creates band tailing and creates voltage deficit. By replacing Cu in CZTSe with isovalent Ag, whose ionic radius is larger than that of Cu and Zn, the density of I-II antisite defects could be suppressed. This work has been done to quantify the cation disorders on all cation symmetry sites and the effect of substitution of Ag in the CZTSe crystal structure. (Ag_xCu_{1-x})₂ZnSnSe₄ (A/CZTSe) samples with different compositions were synthesized by a solid-state reaction of the pure element in an evacuated quartz tube. Structural analysis of stoichiometric & off- stoichiometric samples were performed using Raman and synchrotron powder diffraction including Rietveld refinement. A neutron diffraction experiment is performed to fully understand the cation distribution analysis in A/CZTSe powder sample as Cu⁺ and Zn²⁺ are not distinguishable using conventional X-ray diffraction method due to their isoelectronic character but there is a significant difference in their neutron scattering length ($b_{\text{Cu}} = 7.718 \text{ fm}$, $b_{\text{Zn}} = 5.680 \text{ fm}$). It is found that powder A/CZTSe adopts the kesterite type structure with a partial disorder of copper and zinc on the two Wyckoff position 2c and 2d. Sn has been found on Wyckoff position 2b (0, 0, $\frac{1}{2}$), whereas Cu/Zn is located on 2a (0, 0, 0), 2c (0, $\frac{1}{2}$, $\frac{1}{4}$) and 2d (0, $\frac{1}{2}$, $\frac{3}{4}$) sites. There is a presence of copper vacancies (VCu), various cation anti-site defects (CuZn, ZnCu, ZnSn, and SnZn) have been found for different compositions. This work will also answer the effectiveness of Ag as a substitution of Cu in kesterite based CZTSe, to suppress anti-site disorder.

Abstract ID # 82
Advanced Materials

Shaham Quadir

Upgrades to the Kowari sample positioning system

This poster will highlight some recent additions to improving the spatial positioning of samples on the Kowari instrument for residual stress measurement. This includes cross laser reference point positioning at both 45 and minus 45 degree to the primary beam. In addition the new ATOS GOM structured light scanning system will be described with a brief description on how this may allow live sample tracking to allow for in-situ positioning error correction.

*Abstract ID # 113
Neutron Instruments &
Techniques*

Mark Reid

A structural and magnetic investigation of the skyrmion host material doped Cu₂OSeO₃

A skyrmion is a topologically protected particle-like magnetic spin structures on the order of 10-100 nm. Recent studies have also shown that the skyrmions can be manipulated through applications such as an external electric fields and heat. This offers the potential for development for a much more stable, energy efficient and faster storage in memory devices. The magnetic skyrmions pack into a hexagonal lattice with the skyrmion lattice only stable in a narrow magnetic field-temperature range.^{1–2} Here we present structural analysis of Cu₂OSeO₃ and Te-doped Cu₂OSeO₃ using neutron and x-ray diffraction. A magnetic field-temperature phase diagram mapping of both Cu₂OSeO₃ and Te-doped Cu₂OSeO₃ was also achieved using small angle neutron scattering. Mapping of the magnetic field-temperature phase diagram showed that tellurium doping resulted in an enlarged stability range for the skyrmion phase had been achieved.³

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*Abstract ID # 107
Chemistry &
Crystallography*

Rosanna Rov

Taipan – recent results from the thermal spectrometer at ANSTO

The Australian Centre for Neutron Scattering at ANSTO hosts a suite of four inelastic neutron spectrometers for investigating dynamics in materials over a variety of energy scales (up to 200 meV) and energy resolutions (down to 1 μ eV). The thermal spectrometer, Taipan, has operated as a triple-axis spectrometer since 2010, and more recently from 2016 it has also incorporated an alternative secondary spectrometer, a beryllium filter analyser spectrometer.

We will describe the capabilities of Taipan and present some recent scientific highlights. From this we hope to show the versatility of Taipan for measuring both elastic and inelastic data for samples under a wide range of sample environment conditions.

*Abstract ID # 44
Neutron Instruments &
Techniques*

Kirrily Rule

Scaling behaviour of the skyrmion phases of Cu₂OSeO₃ single crystals from small angle neutron scattering

A skyrmion is a topological stable particle-like object comparable to a spin vortex at the nanometre scale. It consists of an about 50 nm large spin rotation and its spin winding number is quantised. Skyrmions emerge in chiral crystals as the result of competing symmetric exchange and asymmetric Dzyaloshinskii-Moriya (DM) interactions and typically form two dimensional hexagonal lattices perpendicular to an applied magnetic field. Its dynamics has links to flux line vortices as in high-temperature superconductors [1-2].

Cu₂OSeO₃ is a unique case of a multiferroic material where the skyrmion dynamics could be controlled through the application of an external electric field. The direct control of the skyrmion dynamics through a non-dissipative method would offer technological benefits applicable in energy-efficient data storage and data processing devices or for testing fundamental theories also related to the Higgs Boson whose theoretical description has similarities to skyrmions [3].

The technological applications crucially depend on the stability conditions of the skyrmion phase up to room temperature. While some materials host skyrmion lattices above room temperature [3], Cu₂OSeO₃ is the only insulating skyrmion material discovered so far, which orders magnetically below 58 K. It is interesting to note that the appearance of two different skyrmion phases have been reported along the temperature and magnetic field phase diagram of Cu₂OSeO₃ when the sample is aligned with its main crystallographic axes parallel to the incoming neutron beam and performing Zero Field Cooling (ZFC) or Field Cooling (FC) across the high-temperature skyrmion phase. However, the stabilisation processes of these two phases and their thermodynamic connection are still under debate [4-6]. We have used small angle neutron scattering and Lorentz transmission electron microscopy [7] to study the scaling behaviour of helical phase and the magnetic skyrmion lattices, i.e. the systematic change of their distances in single crystals of Cu₂OSeO₃ in order to gain insight on the balance between the different competing magnetic exchange interactions.

Therefore, we have examined the field, temperature and sample alignment dependence of the scaling behaviour of skyrmions as an order parameter for the emergence of the two aforementioned skyrmion phases. The obtained data provide valuable information on the formation mechanism of the skyrmions and their stability range. This is an important step towards the understanding of the manipulation of skyrmions, which is required for technological applications.

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Abstract ID # 87
Magnetism &
Condensed Matter

**Jorge Arturo
Sauceda Flores**

QCM-D and Neutron Reflectometry Study of Effect of Plasma Treatment on Cellulose-Mucin Interactions Towards ETSA

Epidemic thunderstorm asthma (ETSA)[1] is associated with inhalation of airborne pollen grains and aerosolized pollen fragments, causing hypersensitive immune reactions[2] that might lead to an asthma attack. The wall of pollen grains (intine) contains cellulose which is hypothesized to initially interact with the nasal and tracheal mucous layer[3] when inhaled. The air-way mucous layer is comprised of mucin (a major glycosylated proteinaceous element) and water, which serves as a first-line-of-defence against inhaled pollen particles. Although immunological and meteorological studies have been conducted in this regard, the fundamental cause and mechanism of ETSA are under-investigated. This study is focused on unraveling inherent cellulose-mucin interactions employing quartz crystal microbalance with dissipation (QCM-D) and neutron reflectometry (NR) examining the adsorption of mucin on cellulose while mimicking a thunderstorm environment, such as the effect of plasma treatment on cellulose-mucin interactions. Here, we generate air-plasma and plasma-activated water to treat our model cellulose surfaces[4], simulating the ionized surface chemistry of thunderstorm-borne pollen particles and examine subsequent interactions.

In this poster, we describe the use of QCM-D and NR to investigate cellulose-mucin interactions and the effect of plasma treatment on these biointerfacial interactions. The advanced molecular and structural data obtained from this study, coupled with immunological and meteorological investigations, will enable the mechanistic understanding, treatment, and prevention of ETSA.

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Abstract ID # 57
Biological Systems

Arslan Siddique

ANSTO for more than ten years successfully operates Small Angle Neutron Scattering (SANS) instrument Quokka [1] and in 2016 commenced user operation of the second SANS instrument, Bilby [2]. Ultra-small angle scattering machine Kookaburra [3] is completing the set of the SANS instruments at ANSTO.

Bilby exploits neutron Time-of-Flight (ToF) to extend the measurable Q-range, over and above what is possible on a conventional reactor-based monochromatic SANS instrument. In ToF mode, the choppers are used to create neutron pulses of variable ($\sim 3\% - 30\%$) wavelength resolution.

Two arrays of position-sensitive detectors in combination with utilizing of wide wavelength range provide the capability to collect scattering data of wide angular diapason without changing the experimental set-up (maximum accessible Q on the instrument is $0.001-1.8\text{\AA}^{-1}$). Additionally to the ToF, Bilby can operate in monochromatic mode.

The question is how the advanced design features can be applied to the real scientific questions.

In short, having a large dynamic range available in one go opens up a possibility to study complex systems like micelles and hierarchical materials. Additionally, there is a range of sample environments available allowing to change conditions in situ, which is priceless for study a range of samples stretching from colloids to metals.

In my presentation, I will be giving several examples demonstrating how ToF SANS can bring light to structural changes of the surfactant wormlike micelles structure under various conditions.

Some cases will be presented to show that the monochromatic mode is also the one producing valuable results.

The main accent will be made on a recently published work, done solely on Bilby along with examples of combining SANS and USANS techniques.

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*Abstract ID # 103
Neutron Instruments &
Techniques*

Anna Sokolova

Synthesis of New Cuprate's through High Pressure Chemical Vapour Transport

Chemical vapour transport (CVT) reactions has allowed for the growth of many inorganic single crystals which would be difficult or completely impossible to grow using alternative methods like flux related methods or from congruent melt. Most CVT reactions are done in evacuated and sealed quartz tubes where the internal pressure is typically in the range from 1 to 10^{-3} bar where diffusion is the dominant contributor to transport kinetics.[1] Diffusion limited transport is preferred over convective transport because it minimises nucleation, favouring the growth of larger single crystals with fewer defects.

Many metal oxides are simply not thermodynamically stable under these conditions making it difficult to transport and crystallise the desired phase or composition. We have found this to be the case for many cuprates with the braunite, parwelite and various Cu_3TeO_6 related structures. To circumvent this limitation we have explored the unconventional high pressure CVT (HPCVT) method. As a result of these experiments we have been able to successfully grow and solve the structures of single crystals of new polymorphs and structures, this includes $\text{Cu}_5\text{Sb}_2\text{SiO}_{12}$, $\text{Cu}_4\text{MnSb}_2\text{SiO}_{12}$, $\text{Cu}_2\text{GaSbO}_6$ and $\text{Cu}_3\text{Ga}_3\text{SbSiO}_{12}$. Samples have been characterised by X-ray and neutron diffraction and magnetic susceptibility measurements. These structures exhibit exotic gallium and copper coordination environments making them suitable candidates for studying various magnetic phenomena.

HPCVT is a useful method not only for the growth of new inorganic compounds but also as an alternative, environmentally friendly method for growing known structures. Under pressure, water seems to be a major contributor to the transport reaction making it possible to grow samples without a reliance on halogens or commonly used salts like HgBr or TeCl_4 . Since the transport rates are high as a result of greater convective currents, a significantly smaller temperature gradient is necessary to conduct the experiments making much simpler experimental designs possible and accessible without the need for multi-zone furnaces.

[1] Binnewies, M.; Glaum, R.; Schmidt, M.; Schmidt, P. Chemical Vapor Transport Reactions. 2012.

*Abstract ID # 36
Chemistry &
Crystallography*

Martin Spasovski

Opportunities for Catalysis Studies using the Beryllium Filter Spectrometer

The Beryllium Filter Spectrometer (BeF) is one of the inelastic neutron spectrometers located on Taipan, the other being a classical thermal triple axis spectrometer (TAS). The BeF is ideal for vibrational spectroscopy investigations on a molecular level. In particular as the total scattering cross-section of hydrogen is about 82 barn, which is mainly due to incoherent nuclear scattering from the protium isotope, neutron spectroscopy is incredibly sensitive to hydrogen vibrations that can be interpreted on a localised molecular level, over and above most scattering from other isotopes. With this in mind and given the experience gained in successfully using the BeF spectrometer over the last three years, a review of catalysis work is presented that have involved such filter-based spectrometers. In particular studies focusing on hydrogen are highlighted. One of the overarching goals of catalytic studies is the elucidation of structure-function relationships which neutron spectroscopy in Australia could significantly contribute to using the filter spectrometer on Taipan.

*Abstract ID # 84
Neutron Instruments &
Techniques*

Anton Stampfl

Wombat – the high intensity diffractometer at OPAL

Wombat is a high intensity neutron diffractometer located in the OPAL Neutron Guide Hall. It is primarily used as a high-speed powder diffractometer, but has also expanded into texture characterisation and single-crystal measurement. The high performance comes from the combination of a high speed area detector with a large beam guide and correspondingly large crystal monochromator. Wombat can also operate with polarization/analysis.

Wombat has been used to explore a broad range of materials, including: novel hydrogen-storage materials, negative-thermal-expansion materials, methane-ice clathrates, piezoelectrics, high performance battery anodes and cathodes, high strength alloys, multiferroics, superconductors and novel magnetic materials. Our poster will highlight both the capacity of the instrument, and some recent results.

*Abstract ID # 93
Neutron Instruments &
Techniques*

Andrew Studer

In situ diagnostics and optimization of single crystal compound scintillator and semiconductor materials through energy-resolved neutron imaging

The high cost, low yield and inconsistency of crystal growth are among the main obstacles for the introduction of new materials to widespread application in various detection devices. In-situ diagnostics during crystal growth can be very helpful for the optimization of the growth process of a specific material. Neutrons appear to be unique probes providing information on the distribution of elements via nuclear resonance absorption, location of liquid/solid interfaces via different contrasts between elements and some information on the crystallographic structure (such as mosaicity) via Bragg scattering. Recent development of in-situ neutron imaging technique conducted at pulsed neutron sources demonstrate the possibility to visualize in real time (in crystal growth terms) the location of the liquid/solid interface, uniformity of crystal orientation and lattice parameter as well as elemental distribution. In this paper we demonstrate how crystal growth parameters can be optimized in-situ allowing substantial reduction of time required for the optimization of growth conditions. We performed in-situ imaging during crystal growth of several gamma scintillator materials: BaBrCl:Eu, Cs₂LiLaBr₆:Ce, CsI:Eu and others. These crystals were grown by the Bridgman process performed within a dedicated furnace, designed specifically for neutron imaging. Our experiments demonstrate the unique capabilities of energy-resolved neutron imaging to measure various characteristics of crystal growth process with sub-mm spatial resolution and with a ~minute timing resolution, sufficient for slow crystal growth processes.

*Abstract ID # 26
Neutron Instruments &
Techniques*

Anton Tremsin

4d Transition-Metal Substitution into magnetically frustrated A1B3Si2Sn7O16 structures

Includes an overview of the A1B3Si2Sn7O16 (A=Fe, B=Fe,Mn) structural family and it's bi-layered structure, containing both a magnetically frustrated oxide layer and a non-magnetic FeSn6 cluster layer. It then covers the substitution of Fe with Ru in cluster layer and the effect this has on it's magnetic structure, analysed using NPD, with comparison to the effect of other substitution schemes that have been performed on different structural sites.reid

*Abstract ID # 92
Magnetism &
Condensed Matter*

Joseph Vella

Neutron scattering unravels the structure of tunable fibrin networks

Three-dimensional (3D) in vitro cell culture in natural hydrogels has shown promising results in tissue engineering and biophysics as it mimics the native extracellular matrix [1]. However, compared to biosynthetic materials, the often uncontrollable and unstable structural and mechanical properties of natural hydrogels have hindered their wide use. Fibrin is a natural fibrous material that has drawn much interest in tissue engineering and has been employed as a scaffold for 3D cell culture because of its inherent advantages. Yet, the batch-to-batch variation, rapid degradation, uncontrollable structural and mechanical properties are the main shortcomings [2]. To overcome these shortcomings, we have established a new well-defined fibrin network with tuneable architecture and mechanical properties by employing two potent recombinant snake venom proteins. Firstly, a Procoagulant Snake Venom Protein (PSVP), which rapidly activates the thrombin precursor prothrombin, is employed for fibrin network formation; a second recombinant snake venom protein, Anti-fibrinolytic Snake Venom Protein (ASVP) is also utilized to control the fibrin degradation. Initially, confocal laser scanning fluorescence microscopy (CLSM) was employed to characterize the micro-scale structural properties. However, while CLSM can provide detailed information about the network structure, the optical resolution of CLSM is not sufficient to visualize the internal structure of individual fibers. Moreover, the fluorophores that are required for the detection can potentially interfere with the fibrin polymerization. Therefore, we utilised combined small angle neutron scattering (SANS) and ultra-small angle neutron scattering (USANS) techniques to characterize and verify our new defined fibrin network system including internal structure of the individual fibres and the structure of the fibrin networks [3].

The combined SANS and USANS data of fibrin networks revealed details of the hierarchical structure at multiple length scales associated with the network, fibres and internal proto-fibrils, previously not accessible by CLSM, especially in the case of internal fibre structure. This data is key for correlating the network structure and the mechanical properties, which are fundamental for cellular responses including cell proliferation, migration and differentiation.

*Abstract ID # 34
Advanced Materials*

Zhao Wang

The ANSTO contribution to a project to provide experimental standards for SAS profile prediction

The program CRY SOL1, was the first method developed to rapidly calculate small-angle scattering (SAS) profiles from atomic coordinates of biomolecules. It was a major breakthrough, providing the missing link between high-resolution structures and solution SAS data. The importance of this breakthrough is evident in the fact that decades later, alternate methods continue to be published with various claims of improvement.

To date, each of the alternate methods published have been validated using different data sets and models. A consensus set of high quality data would be of considerable value in benchmarking the different approaches. In order to evaluate different approaches to including the hydration layer contribution to the SAS profile, it is desirable to have data obtained using X-rays (SAXS) and neutrons (SANS), the latter in H₂O and D₂O, as the hydration layer contribution differs significantly for each of these measurements.

To develop a consensus set of high quality data, an international project involving the efforts of 37 researchers from 11 different X-ray and 3 different neutron scattering facilities across Asia, Europe and North America was undertaken. Here, we report on the contribution of ANSTO to this international project.

1Svergun (1995) J. Appl. Cryst. 28:768

*Abstract ID # 102
Biological Systems*

Andrew Whitten

Quokka, the Pinhole Small-Angle Neutron Scattering Instrument at ANSTO

Quokka was the first Small Angle Neutron Scattering instrument to be in operation at the Australian research reactor, OPAL [1]. It is a 40 m pinhole instrument operating with a neutron velocity selector, an adjustable collimation system providing source-sample distances of up to 20 m and a two dimensional 1 metre square position-sensitive detector, capable of measuring neutrons scattered from the sample over a secondary flight path of up to 20 m. Also offering incident beam polarization and analysis capability as well as lens focusing optics, Quokka has been designed as a general purpose SANS instrument with a large sample area, capable of accommodating a variety of sample environments. Calibrated absolute scattering intensity measurements in a standard setup may be made over a range of wavelengths between $4 \times 10^{-3} \text{ \AA}^{-1}$ and 0.7 \AA^{-1} .

Here we describe Quokka's design characteristics, performance and operation, including a high count rate detector, installed in 2018. Outputs from Quokka have been published in diverse fields such as magnetism, metallurgy, mineralogy, structural biology, polymers, food science and soft matter. We present here a selection of recent scientific highlights.

[1] K. Wood [...] and G. Elliot, J. Appl. Cryst. 51 (2018) 294.

*Abstract ID # 114
Neutron Instruments &
Techniques*

Kathleen Wood

Composition and temperature dependent structural investigation of perovskite-type sodium-ion solid electrolyte series $\text{Na}_{1/2-x}\text{La}_{1/2-x}\text{Sr}_2\text{ZrO}_3$

The development of new solid electrolytes is becoming increasingly important, e.g. in rechargeable batteries for electric vehicles, where current organic electrolytes cause major safety concerns. The ABO_3 perovskite metal oxides have shown excellent lithium and sodium ion conductivity owing to their stability and structural flexibility. This has led to the development of several perovskite-type solid electrolytes such as $\text{Li}_3\text{xLa}_{2/3-x}\text{TiO}_3$ and $\text{Na}_{1/2-x}\text{La}_{1/2-x}\text{Sr}_2\text{ZrO}_3$, which have shown high ionic conductivity.

The $\text{Na}_{1/2-x}\text{La}_{1/2-x}\text{Sr}_2\text{ZrO}_3$ perovskite-type sodium-ion solid electrolyte system was recently published by Zhao et al. [1] with the $x=1/6$ member, i.e. $\text{Na}_{1/3}\text{La}_{1/3}\text{Sr}_{1/3}\text{ZrO}_3$, found to have the highest ionic conductivity. The structure was reported to adopt a cubic crystal system with the space group $\text{P}213$. However, this is highly unlikely as both theoretical end members of the series, $\text{Na}_{1/2}\text{La}_{1/2}\text{ZrO}_3$ and SrZrO_3 , have orthorhombic symmetry[2, 3]. Given the high ionic conductivity reported for the system, it is important to determine its structure reliable and with the best available data. Using neutron and X-ray powder diffraction data we have been able to confirm that the symmetry across the series is lowered to orthorhombic indeed. Variable temperature neutron powder diffraction data collected for the $x=1/6$ member of the system from room temperature to 1100 °C helped to identify a structural phase transition from orthorhombic to tetragonal symmetry at 800 °C.

[1] Y.Z. Zhao, Z.Y. Liu, J.X. Xu, T.F. Zhang, F. Zhang, X.G. Zhang, Synthesis and characterization of a new perovskite-type solid-state electrolyte of $\text{Na}_{1/3}\text{La}_{1/3}\text{Sr}_{1/3}\text{ZrO}_3$ for all-solid-state sodium-ion batteries, *J Alloy Compd*, 783 (2019) 219-225.

[2] B.J. Kennedy, C.J. Howard, B.C. Chakoumakos, High-temperature phase transitions in SrZrO_3 , *Phys Rev B*, 59 (1999) 4023-4027.

[3] M.C. Knapp, P.M. Woodward, Ohio State University. Department of Chemistry, Investigations into the structure and properties of ordered perovskites, layered perovskites, and defect pyrochlores, in, Ohio State University,, Columbus, Ohio, 2006, pp. xvii, 161 p.

Abstract ID # 69
Chemistry &
Crystallography

Frederick Yang

Recent highlights from the cold-neutron triple-axis spectrometer SIKA

In this presentation, we will show the Taiwanese built cold-neutron triple-axis spectrometer SIKA at ACNS which was funded by the Ministry of Science and Technology (MoST), Taiwan. We are now running the user program since 2015 with over 20 papers published since then. The cold-neutron triple-axis spectrometer SIKA excels at measuring well-defined regions in $S(Q, \omega)$ space with very low background allowing for parametric studies (eg varying temperature or magnetic field) to be conducted efficiently. Also, triple-axis spectrometers have the advantage of accommodating a wide variety of sample environments and operating with polarized neutrons for both inelastic and elastic scattering experiments. Triple axis spectrometers have been one of the most versatile neutron scattering instruments for many areas of neutron science. The cold neutrons available at SIKA allow us to investigate physical phenomena with high energy and momentum resolution. With other inelastic scattering instruments PELICAN, EMU, and TAIPAN in ACNS, ACNS can cover a large area of $S(Q, \omega)$ space of your research.

We will outline the components, capabilities, sample environment, software, and statistics of SIKA. We will present some of our recent scientific highlights from SIKA since the last AANSS2018. Finally, we will present the current instrument developments on SIKA to accommodate ^3He Polarization analysis. Polarized neutrons can help users to study the properties of materials from proteins to quantum magnets in greater detail.

*Abstract ID # 23
Neutron Instruments &
Techniques*

Shinichiro Yano

Neutron Study of Magnetic Phase Transition in SrCoO₃ Thin Films

Transition metal oxides represent a wide set of materials with a broad range of functionalities which can be tuned by the careful choice of parameters such as strain, oxygen content, and applied electric or magnetic fields. When the material exhibits more than one primary ferroic ordering- ferromagnetism, ferroelectricity, ferroelasticity or ferrotoridicity in the same phase, it becomes multiferroic. Such class of materials are of immense technological interest as magnetic and electric transitions can be driven through external factors. This opens new avenues for fundamental research and technical applications in spintronic or magnonic devices. Here, we present results we obtained from neutron-based techniques to investigate the magnetic properties of SrCoO₃ and similar thin films.

SrCoO₃ provides a particularly interesting system for these investigations. Lee and Rabe have simulated the effect of strain and have predicted that the magnetic state can be tuned through compressive or tensile strain with a ferromagnetic-antiferromagnetic phase transition. Such a phase transition would be accompanied by a metal-to-insulator phase transition and a transition to a ferroelectric polarized state.

By using different substrates, we investigated the effect different epitaxial strain has on SrCoO₃ thin films. Previously, our neutron diffraction experiments on these 40 nm thin films have confirmed the predicted but hitherto unobserved phase transition from ferromagnetism to G-type antiferromagnetism when the film was grown on SrTiO₃ and DyScO₃ substrate respectively. As such, SrCoO₃ would constitute a new class of multiferroic material where magnetic and electric polarizations can be driven through external strain. This tunability makes them ideal candidate materials for use in developing novel information and energy technologies.

*Abstract ID # 72
Advanced Materials*

Samuel Yick

Recent scientific highlights from the Pelican user programme

The direct geometry, time-of-flight spectrometer Pelican has been in the user programme since October 2014 at the OPAL research reactor at the Australian Nuclear Science and Technology Organisation (ANSTO). Situated on the cold guide CG1, Pelican is suited to measuring low energy excitations from varying materials. This encompasses phenomena that are as diverse as the diffusion of water in clays to the observation of crystal field splitting in rare earth magnets. In the current contribution we will highlight some of the recent work that has used Pelican including experiments that use our available range of sample environment equipment which includes dilution temperatures, gas and vapour delivery, a high temperature furnace and a conventional cryostat.

*Abstract ID # 39
Neutron Instruments &
Techniques*

Dehong Yu

PELICAN –a Time of Flight Cold Neutron Spectrometer – New Capabilities

The time-of-flight direct-geometry neutron spectrometer, Pelican, has been in user programme since 2014 at the OPAL research reactor, at the Australian Nuclear Science and Technology Organisation (ANSTO). The Pelican instrument was designed to meet the diverse requirements of the Australian scientific community from physics, chemistry, material science, to biology. A wide range of research fields is covered. These include crystal-field excitations, phonon densities of states, magnetic excitations for various multifunctional materials including high T_c superconductors, novel magnetic, thermoelectric, ferroelectric and piezoelectric materials; molecular dynamics in hydrogen-bonded and storage materials, catalytic materials, cements, soils and rocks; and water dynamics in proteins and ion diffusion in membranes. Polarized neutrons and polarisation analysis option makes the full use of the neutron spin to study magnetism and to separate the coherent and incoherent scatterings.

To cover the broad range of scientific fields, a series of sample environment equipment has been developed. These include a standard cryofurnace capable of providing sample temperature from 1.5 K to 800 K, and special sample environments such as gas sorption, light irradiation, electric fields and dilution temperatures at 50 mK. Recently, we have further extended the instrument capabilities to high magnetic fields up to 7 T, a fast dilution system reaching 10 mK, and a high pressure cell suitable for pressures up to 2 GPa. These new sample environment capabilities have opened up new scientific opportunities on the instrument. In this presentation, we shall describe the performance of the new equipment and the potential new science associated with them.

*Abstract ID # 40
Neutron Instruments &
Techniques*

Dehong Yu

Deciphering the quaternary structure of PEDOT:PSS solution by combining SAXS and SANS characterizations

Poly(3,4-ethylenedioxythiophene) (PEDOT) is a widely used conductive polymer material for organic thermoelectric device, stretchable bioelectronics, optoelectronics and so on. Its success is largely attributed to the availability of the polymer dispersion. Recently people try to decipher the highly conductive nature of the PEDOT:PSS hybrid from molecular assembly with structural hierarchy. Meanwhile, a quaternary structure is well recognized in the complex systems like proteins, and it plays crucial roles in determining the protein functionality. Small angle scattering is a widely employed technique for the structural deciphering of protein solution. In this presentation, we will introduce our recent work on deciphering the quaternary structure of PEDOT:PSS solution based on the combined SAXS and SANS data.

*Abstract ID # 21
Chemistry &
Crystallography*

Peng Zhan